```
Connecting via Winsock to STN



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TERMINAL (ENTER 1, 2, 3, OR 7):2


* * * * * * * * * *   Welcome to STN International   * * * * * * * * * *

 NEWS  1          Web Page for STN Seminar Schedule - N. America
 NEWS  2  JAN 08  CHEMLIST enhanced with New Zealand Inventory of Chemicals
 NEWS  3  JAN 16  CA/CAplus Company Name Thesaurus enhanced and reloaded
 NEWS  4  JAN 16  IPC version 2007.01 thesaurus available on STN
 NEWS  5  JAN 16  WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
 NEWS  6  JAN 22  CA/CAplus updated with revised CAS roles
 NEWS  7  JAN 22  CA/CAplus enhanced with patent applications from India
 NEWS  8  JAN 29  PHAR reloaded with new search and display fields
 NEWS  9  JAN 29  CAS Registry Number crossover limit increased to 300,000 in
                  multiple databases
 NEWS 10  FEB 15  PATDPASPC enhanced with Drug Approval numbers
 NEWS 11  FEB 15  RUSSIAPAT enhanced with pre-1994 records
 NEWS 12  FEB 23  KOREAPAT enhanced with IPC 8 features and functionality
 NEWS 13  FEB 26  MEDLINE reloaded with enhancements
 NEWS 14  FEB 26  EMBASE enhanced with Clinical Trial Number field
 NEWS 15  FEB 26  TOXCENTER enhanced with reloaded MEDLINE
 NEWS 16  FEB 26  IFICDB/IFIPAT/IFIUDB reloaded with enhancements
 NEWS 17  FEB 26  CAS Registry Number crossover limit increased from 10,000
                  to 300,000 in multiple databases
 NEWS 18  MAR 15  WPIDS/WPIX enhanced with new FRAGHITSTR display format
 NEWS 19  MAR 16  CASREACT coverage extended
 NEWS 20  MAR 20  MARPAT now updated daily
 NEWS 21  MAR 22  LWPI reloaded
 NEWS 22  MAR 30  RDISCLOSURE reloaded with enhancements
 NEWS 23  APR 02  JICST-EPLUS removed from database clusters and STN
 NEWS 24  APR 10  GENBANK reloaded and enhanced with Genome Project ID field
 NEWS 25  APR 10  CHEMCATS enhanced with 1.2 million new records
 NEWS 26  APR 30  CA/CAplus enhanced with 1870-1889 U.S. patent records
 NEWS 27  APR 30  INPADOC replaced by INPADOCDB on STN
 NEWS 28  MAY 01  New CAS web site launched
 NEWS 29  MAY 08  CA/CAplus Indian patent publication number format defined
 NEWS 30  MAY 14  RDISCLOSURE on STN Easy enhanced with new search and display
                  fields
 NEWS 31  MAY 21  BIOSIS reloaded and enhanced with archival data
 NEWS 32  MAY 21  TOXCENTER enhanced with BIOSIS reload
 NEWS 33  MAY 21  CA/CAplus enhanced with additional kind codes for German
                  patents
 NEWS 34  MAY 22  CA/CAplus enhanced with IPC reclassification in Japanese
                  patents

 NEWS EXPRESS  NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT
               MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN    Welcome Banner and News Items
```



```
 NEWS IPC8     For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that
specific topic.

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* * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 09:24:16 ON 23 MAY 2007

=> file reg
COST IN U.S. DOLLARS                                 SINCE FILE      TOTAL
                                                        ENTRY     SESSION
FULL ESTIMATED COST                                      0.21        0.21

FILE 'REGISTRY' ENTERED AT 09:24:23 ON 23 MAY 2007
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   22 MAY 2007  HIGHEST RN 935655-41-7
DICTIONARY FILE UPDATES:  22 MAY 2007  HIGHEST RN 935655-41-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10.572772\no bonds.str
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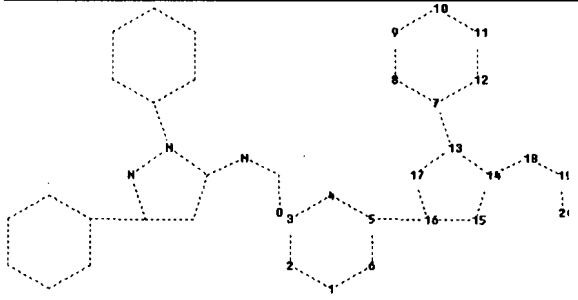


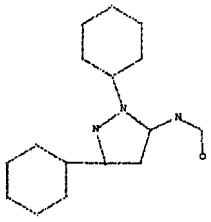

```
chain nodes :
18  19  20
ring nodes :
1  2  3  4  5  6  7  8  9  10  11  12  13  14  15  16  17
chain bonds :
5-16  7-13  14-18  18-19  19-20
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  7-8  7-12  8-9  9-10  10-11  11-12  13-14  13-17  14-15
15-16  16-17
exact/norm bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-16  7-8  7-12  7-13  8-9  9-10  10-11  11-12  13-14
13-17  14-15  14-18  15-16  16-17  18-19  19-20


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:Atom  13:Atom  14:Atom  15:Atom  16:Atom  17:Atom  18:CLASS  19:CLASS  20:CLASS



L1      STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1              STR
```


```
Structure attributes must be viewed using STN Express query preparation.


=> s l1 sss sam
SAMPLE SEARCH INITIATED 09:24:56 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -        91 TO ITERATE

100.0% PROCESSED       91 ITERATIONS                                 24 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          1248 TO     2392
PROJECTED ANSWERS:              187 TO      773

L2            24 SEA SSS SAM L1

=> d scab
'SCAB' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual
fields or predefined formats.  The predefined substance formats
are:  (RN = CAS Registry Number)

REG     - RN
SAM     - Index Name, MF, and structure - no RN
FIDE    - All substance data, except sequence data
IDE     - FIDE, but only 50 names
SQIDE   - IDE, plus sequence data
SQIDE3  - Same as SQIDE, but 3-letter amino acid codes are used
SQD     - Protein sequence data, includes RN
SQD3    - Same as SQD, but 3-letter amino acid codes are used
SQN     - Protein sequence name information, includes RN

CALC    - Table of calculated properties
EPROP   - Table of experimental properties
PROP    - EPROP and CALC

Any CA File format may be combined with any substance format to
obtain CA references citing the substance.  The substance formats
```

must be cited first. The CA File predefined formats are:

ABS -- Abstract
APPS -- Application and Priority Information
BIB -- CA Accession Number, plus Bibliographic Data
CAN -- CA Accession Number
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)
IND -- Index Data
IPC -- International Patent Classification
PATS -- PI, SO
STD -- BIB, IPC, and NCL

IABS -- ABS, indented, with text labels
IBIB -- BIB, indented, with text labels
ISTD -- STD format, indented

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.
The MAX format is the same as ALL.
The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields.
HELP FORMATS -- To see detailed descriptions of the predefined formats.
ENTER DISPLAY FORMAT (IDE):d scan
'D' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

REG - RN
SAM - Index Name, MF, and structure - no RN
FIDE - All substance data, except sequence data
IDE - FIDE, but only 50 names
SQIDE - IDE, plus sequence data
SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used
SQD - Protein sequence data, includes RN
SQD3 - Same as SQD, but 3-letter amino acid codes are used
SQN - Protein sequence name information, includes RN

CALC - Table of calculated properties
EPROP - Table of experimental properties
PROP - EPROP and CALC

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

ABS -- Abstract
APPS -- Application and Priority Information
BIB -- CA Accession Number, plus Bibliographic Data

CAN -- CA Accession Number
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)
IND -- Index Data
IPC -- International Patent Classification
PATS -- PI, SO
STD -- BIB, IPC, and NCL

IABS -- ABS, indented, with text labels
IBIB -- BIB, indented, with text labels
ISTD -- STD format, indented

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

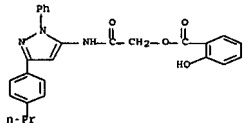
The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.
The MAX format is the same as ALL.
The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields.
HELP FORMATS -- To see detailed descriptions of the predefined formats.
ENTER DISPLAY FORMAT (IDE):end

=> d scan

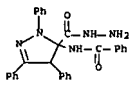
L2 24 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Benzoic acid, 2-hydroxy-, 2-oxo-2-[[1-phenyl-3-(4-propylphenyl)-1H-pyrazol-5-yl]amino]ethyl ester (9CI)
MF C27 H25 N3 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 24 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 1H-Pyrazole-5-carboxylic acid, 5-(benzoylamino)-4,5-dihydro-1,3,4-triphenyl-, hydrazide (9CI)
MF C29 H25 N5 O2

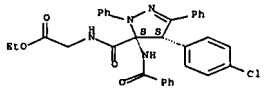


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 24 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Glycine, N-[[5-(benzoylamino)-4-(4-chlorophenyl)-4,5-dihydro-1,3-diphenyl-1H-pyrazol-5-yl]carbonyl]-, ethyl ester, cis- (9CI)
MF C33 H29 Cl N4 O4

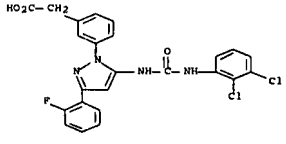
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

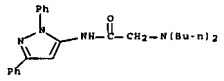
L2 24 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Benzeneacetic acid, 3-[5-[[[(2,3-dichlorophenyl)amino]carbonyl]amino]-3-(2-fluorophenyl)-1H-pyrazol-1-yl]- (9CI)
MF C24 H17 Cl2 F N4 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 24 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Acetamide, 2-(dibutylamino)-N-(1,3-diphenylpyrazol-3-yl)- (8CI)
MF C25 H32 N4 O
CI COM

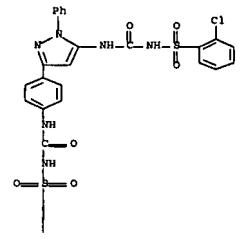


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 24 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Benzenesulfonamide, 2-chloro-N-[[[3-[4-[[[[(2-chlorophenyl)sulfonyl]amino]carbonyl]amino]phenyl]-1-phenyl-1H-pyrazol-5-yl]amino]carbonyl]- (9CI)
MF C29 H22 Cl2 N6 O6 S2

PAGE 1-A



PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> s l1 sss full
FULL SEARCH INITIATED 09:25:41 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1599 TO ITERATE

100.0% PROCESSED 1599 ITERATIONS 413 ANSWERS
SEARCH TIME: 00.00.01

L3 413 SEA SSS FUL L1

=> file hcaplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 172.55 172.76

FILE 'HCAPLUS' ENTERED AT 09:25:46 ON 23 MAY 2007
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FILE COVERS 1907 - 23 May 2007 VOL 146 ISS 22
FILE LAST UPDATED: 22 May 2007 (20070522/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

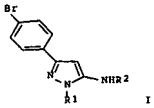
=> s l3
L4 128 L3

=> s l4 and py <2004
23932542 PY <2004
L5 92 L4 AND PY <2004

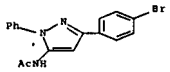
=> d ibib abs hitstr 1-10

L5 ANSWER 1 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:153241 HCAPLUS Full-text
DOCUMENT NUMBER: 141:395467
TITLE: 3-(p-Bromophenyl)-5-aminopyrazole and some derivatives
AUTHOR(S): Nam, N. L.; Grandberg, I. I.; Sorokin, V. I.
CORPORATE SOURCE: Kafedra Org. Khim., Timiryazevsk. S-Kh. Akad., Russia
SOURCE: Izvestiya Timiryazevskoi Sel'skokhozyaistvennoi

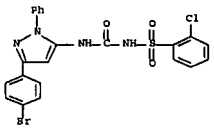
Akademii (2003), (4), 142-146
CODEN: ITSAA7; ISSN: 0021-342X
PUBLISHER: ANO "Izdatel'stvo MSKhA"
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 141:395467
GI



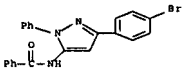
AB 5-Aminopyrazoles I (R1 = H, Me, Ph; R2 = H) were readily prepared via cyanation of α,4-dibromoacetophenone with sodium cyanide followed by heterocyclization of 4-bromo-α-cyanoacetophenone with the corresponding hydrazines. Pyrazole I (R1 = Ph; R2 = H) was further functionalized by reactions with acyl and sulfonyl halides, anhydrides or isocyanates to give I (R1 = Ph; R2 = MeCO, PhCO, 4-MeC6H4SO2, 2-ClC6H4SO2NHCO).
IT 342413-16-5P 786688-48-0P 786688-49-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of (bromophenyl)aminopyrazoles)
RN 342413-16-5 HCAPLUS
CN Acetamide, N-[3-(4-bromophenyl)-1-phenyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)



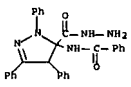
RN 786688-48-0 HCAPLUS
CN Benzenesulfonamide, N-[[[3-(4-bromophenyl)-1-phenyl-1H-pyrazol-5-yl]amino]carbonyl]-2-chloro- (9CI) (CA INDEX NAME)



RN 786688-49-1 HCAPLUS
CN Benzamide, N-[3-(4-bromophenyl)-1-phenyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

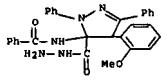


L5 ANSWER 2 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:943836 HCAPLUS Full-text
DOCUMENT NUMBER: 141:243428
TITLE: Synthesis and Reactions of Some New Heterocyclic Carbohydrazides and Related Compounds as Potential Anticancer Agents
AUTHOR(S): Mansour, Abdel Kader; Eid, Mohga M.; Khalil, Nasser S. A. M.
CORPORATE SOURCE: Department of Chemistry, Faculty of Science, Cairo University, Giza, Egypt
SOURCE: Molecules (2003), 8(10), 744-755
CODEN: MOLEFW; ISSN: 1420-3049
URL: http://www.mdpi.org/molecules/papers/81000744.pdf
PUBLISHER: Molecular Diversity Preservation International
DOCUMENT TYPE: Journal; (online computer file)
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:243428
AB Acylation of 3-hydrazino-5,6-diphenyl-1,2,4-triazine and hydrazine hydrate with 4-aryl-1,3,7-triphenyl-8-oxa-1,2,6-triazaspiro[4.4]nona-2,6-dien-9- ones gave the corresponding heterocyclic carbohydrazides. Conversion of some of the later compds. into the versatile carbohydrazide derivs. and the related oxadiazoles was undertaken. A primary in vitro test of one of the products (concentration 10-4 M) showed activity against leukemia cell lines (CCRF-CEM, K-256, MOLT-4, PRMI-8226, SR).
IT 752257-66-2P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation of heterocyclic carbohydrazides and related compds. as potential anticancer agents)
RN 752257-66-2 HCAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 5-(benzoylamino)-4,5-dihydro-1,3,4-triphenyl-, hydrazide (9CI) (CA INDEX NAME)

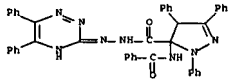


IT 752257-67-3P

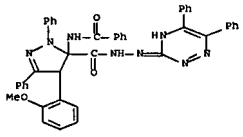
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of heterocyclic carbohydrazides and related compds. as potential anticancer agents)
RN 752257-67-3 HCAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 5-(benzoylamino)-4,5-dihydro-4-(2-methoxyphenyl)-1,3-diphenyl-, hydrazide (9CI) (CA INDEX NAME)



IT 752257-64-0P 752257-65-1P 752257-69-4P
752257-69-5P 752257-70-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of heterocyclic carbohydrazides and related compds. as potential anticancer agents)
RN 752257-64-0 HCAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 5-(benzoylamino)-4,5-dihydro-1,3,4-triphenyl-, 2-(5,6-diphenyl-1,2,4-triazin-3-yl)hydrazide (9CI) (CA INDEX NAME)

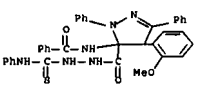


RN 752257-65-1 HCAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 5-(benzoylamino)-4,5-dihydro-4-(2-methoxyphenyl)-1,3-diphenyl-, 2-(5,6-diphenyl-1,2,4-triazin-3-yl)hydrazide (9CI) (CA INDEX NAME)

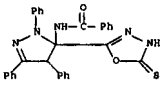


RN 752257-68-4 HCAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 5-(benzoylamino)-4,5-dihydro-4-(2-methoxyphenyl)-1,3-diphenyl-, 2-[(phenylamino)thioxomethyl]hydrazide (9CI)

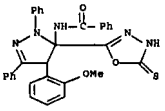
(CA INDEX NAME)



RN 752257-69-5 HCAPLUS
CN Benzamide, N-[5-(4,5-dihydro-5-thioxo-1,3,4-oxadiazol-2-yl)-4,5-dihydro-1,3,4-triphenyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)



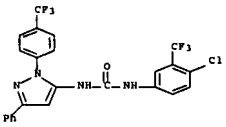
RN 752257-70-8 HCAPLUS
CN Benzamide, N-[5-(4,5-dihydro-5-thioxo-1,3,4-oxadiazol-2-yl)-4,5-dihydro-4-(2-methoxyphenyl)-1,3-diphenyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)



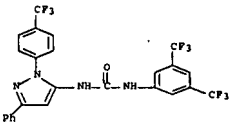
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:928892 HCAPLUS Full-text
DOCUMENT NUMBER: 140:156733
TITLE: Ureas of 5-aminopyrazole and 2-aminothiazole inhibit growth of gram-positive bacteria
AUTHOR(S): Kane, John L.; Hirth, Bradford H.; Liang, Beirong; Gourlie, Brian B.; Nahill, Sharon; Barsomian, Gary
CORPORATE SOURCE: Genzyme Drug Discovery and Development, Genzyme Corp., Cambridge, MA, 02139, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2003), 13(24), 4463-4466
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

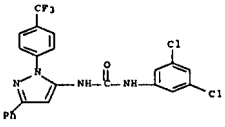
AB Ureas of 5-aminopyrazole and 2-aminothiazole emerged as lead compds. from a high-throughput screen assaying the growth of Staphylococcus aureus. Structure-activity relationships were developed for each compound series. Several compds. were also tested for activity against drug resistant strains of S. aureus in vivo.
IT 438242-75-2 438242-76-3 438242-77-4
438242-92-3 656256-42-7 656256-43-8
656256-44-9 656256-45-0
RL: PAC (Pharmacological activity); BIOL (Biological study)
(ureas of 5-aminopyrazole and 2-aminothiazole inhibit growth of gram-pos. bacteria)
RN 438242-75-2 HCAPLUS
CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[3-phenyl-1-[4-(trifluoromethyl)phenyl]-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)



RN 438242-76-3 HCAPLUS
CN Urea, N-[3,5-bis(trifluoromethyl)phenyl]-N'-[3-phenyl-1-[4-(trifluoromethyl)phenyl]-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

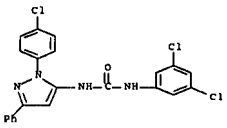


RN 438242-77-4 HCAPLUS
CN Urea, N-(3,5-dichlorophenyl)-N'-[3-phenyl-1-[4-(trifluoromethyl)phenyl]-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

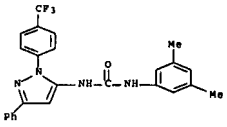


RN 438242-92-3 HCAPLUS

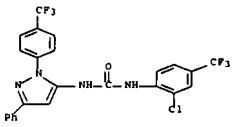
CN Urea, N-[1-(4-chlorophenyl)-3-phenyl-1H-pyrazol-5-yl]-N'-(3,5-dichlorophenyl)- (9CI) (CA INDEX NAME)



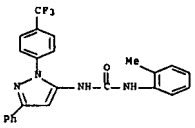
RN 656256-42-7 HCAPLUS
CN Urea, N-(3,5-dimethylphenyl)-N'-[3-phenyl-1-[4-(trifluoromethyl)phenyl]-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)



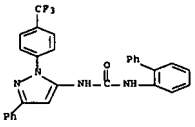
RN 656256-43-8 HCAPLUS
CN Urea, N-[2-chloro-4-(trifluoromethyl)phenyl]-N'-[3-phenyl-1-[4-(trifluoromethyl)phenyl]-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)



RN 656256-44-9 HCAPLUS
CN Urea, N-(2-methylphenyl)-N'-[3-phenyl-1-[4-(trifluoromethyl)phenyl]-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)



RN 656256-45-0 HCAPLUS
CN Urea, N-[1,1'-biphenyl]-2-yl-N'-[3-phenyl-1-[4-(trifluoromethyl)phenyl]-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:826823 HCAPLUS Full-text
DOCUMENT NUMBER: 139:317441
TITLE: 2-(3-Hydroxyanilino)-2-oxoacetamide derivatives and interleukin 12 production inhibitors containing them
INVENTOR(S): Sato, Masakazu; Matsunaga, Yuiko; Ushiki, Yasunobu; Ito, Nobumasa; Nishimura, Koji
PATENT ASSIGNEE(S): Taisho Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 27 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

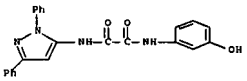
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003300875	A	20031021	JP 2002-106023	20020409 <--
PRIORITY APPLN. INFO.:			JP 2002-106023	20020409

OTHER SOURCE(S): MARPAT 139:317441
AB 3-(HOC6H4)NHCOCONHR [I; R = (un)substituted Ph, (un)substituted naphthyl, (un)substituted pyridyl, quinolinyl, (alkyl)benzothiazolyl, (un)substituted thienyl, (un)substituted pyrazolyl; substituents are given] and their pharmaceutically acceptable salts and interleukin 12 production inhibitors containing I or their salts are claimed. I [R = C6H3(OMe)2-3,4] at 30 μm showed 89.7% inhibition on INF-γ-stimulated production of interleukin 12 by human peripheral blood monocytes.
IT 614722-97-3
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation of 3-hydroxyanilide derivs. [N-(hetero)aryl-N'-

(hydroxyphenyl)oxalamides] as 12 production inhibitors)

RN 614722-97-3 HCAPLUS

CN Ethanediamide, N-(1,3-diphenyl-1H-pyrazol-5-yl)-N'-(3-hydroxyphenyl)- (9CI) (CA INDEX NAME)



L5 ANSWER 5 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:738975 HCAPLUS Full-text

DOCUMENT NUMBER: 139:301299

TITLE: Structure-Activity Relationships of the p38α MAP Kinase Inhibitor 1-(5-tert-Butyl-2-p-tolyl-2H-pyrazol-3-yl)-3-[4-(2-morpholin-4-yl-ethoxy)naphthalen-1-yl]urea (BIRB 796)

AUTHOR(S): Regan, John; Capolino, Alison; Cirillo, Pier F.; Gilmore, Thomas; Graham, Anne G.; Hickey, Eugene; Kroe, Rachel R.; Madwed, Jeffrey; Moriak, Monica; Nelson, Richard; Pargellis, Christopher A.; Swinamer, Alan; Torcellini, Carol; Tsang, Michele; Moss, Neil

CORPORATE SOURCE: Research and Development Center, Department of Medicinal Chemistry, Boehringer Ingelheim Pharmaceuticals, Ridgefield, CT, 06877, USA

SOURCE: Journal of Medicinal Chemistry (2003), 46(22), 4676-4686
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:301299

AB We report on the structure-activity relationships (SAR) of 1-(5-tert-butyl-2-p-tolyl-2H-pyrazol-3-yl)-3-[4-(2-morpholin-4-yl- ethoxy)naphthalen-1-yl]urea (BIRB 796), an inhibitor of p38α MAP kinase which has advanced into human clin. trials for the treatment of autoimmune diseases. Thermal denaturation was used to establish mol. binding affinities for this class of p38α inhibitors. The tert-Bu group remains a critical binding element by occupying a lipophilic domain in the kinase which is exposed upon rearrangement of the activation loop. An aromatic ring attached to N-2 of the pyrazole nucleus provides important π-CH2 interactions with the kinase. The role of groups attached through an ethoxy group to the 4-position of the naphthalene and directed into the ATP-binding domain is elucidated. Pharmacophores with good hydrogen bonding potential, such as morpholine, pyridine, and imidazole, shift the melting temperature of p38α by 16-17° translating into Kd values of 50-100 pM. Finally, we describe several compds. that potently inhibit TNF-α production when dosed orally in mice.

IT 285983-51-2P

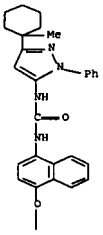
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(synthesis and p38α kinase-inhibiting activity of BIRB 796 analogs for treatment of autoimmune diseases)

RN 285983-51-9 HCAPLUS

CN Urea, N-[3-(1-methylcyclohexyl)-1-phenyl-1H-pyrazol-5-yl]-N'-[4-[2-(4-morpholinyl)ethoxy]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 6 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:656575 HCAPLUS Full-text

DOCUMENT NUMBER: 139:197476

TITLE: Preparation of aryl heterocyclyl ureas with raf kinase and angiogenesis inhibiting activity

INVENTOR(S): Dumas, Jacques; Scott, William J.; Elting, James; Hatoum-Makdad, Holia

PATENT ASSIGNEE(S): Bayer Corporation, USA

SOURCE: PCT Int. Appl., 142 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

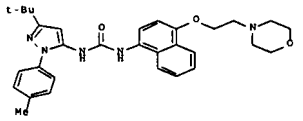
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003068223	A1	20030821	WO 2003-US4102	20030211 <--

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

AU 2003210969	A1	20030904	AU 2003-210969		20030211 <--
US 2004023961	A1	20040205	US 2003-361844		20030211
PRIORITY APPLN. INFO.:			US 2002-354948P	P	20020211
			WO 2003-US4102	W	20030211

GI



I

AB 283 Of the title ureas useful for treating diseases mediated by raf kinase and diseases mediated by the VEGF induced signal transduction pathway characterized by abnormal angiogenesis or hyperpermeability processes, were claimed. Synthesis of 6 ureas such as I was described. Thus, reacting 3-(tert-butyl)-1-(4-methylphenyl)pyrazole-5-ylamine with 4-(2-morpholin-4-ylethoxy)naphthylamine (prepns. given) and CDI in CH2Cl2 afforded 80% I which showed IC50 of < 1 μM in in vitro raf kinase and in in vitro Flk-1 ELISA assay.

IT 285983-51-9P 285983-96-2P

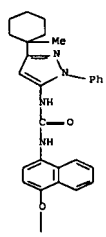
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of aryl heterocyclyl ureas with raf kinase and angiogenesis inhibiting activity)

RN 285983-51-9 HCAPLUS

CN Urea, N-[3-(1-methylcyclohexyl)-1-phenyl-1H-pyrazol-5-yl]-N'-[4-[2-(4-morpholinyl)ethoxy]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

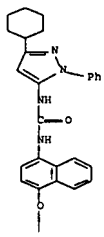


PAGE 2-A

RN 285983-96-2 HCAPLUS

CN Urea, N-(3-cyclohexyl-1-phenyl-1H-pyrazol-5-yl)-N'-[4-[2-(4-morpholinyl)ethoxy]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 7 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:633448 HCAPLUS Full-text
DOCUMENT NUMBER: 139:185666
TITLE: Coated pharmaceutical tablets with speckled appearance
INVENTOR(S): Martino, Alice C.; Noack, Robert M.; Pierman, Steven A.
PATENT ASSIGNEE(S): Pharmacia Corporation, USA
SOURCE: PCT Int. Appl., 30 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003066030	A2	20030814	WO 2003-US3837	20030206 <--
WO 2003066030	A3	20031016		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2474921	A1	20030814	CA 2003-2474921	20030206 <--
AU 2003210930	A1	20030902	AU 2003-210930	20030206 <--
US 2003180357	A1	20030925	US 2003-359939	20030206 <--
EP 1480624	A2	20041201	EP 2003-737712	20030206
EP 1480624	B1	20061129		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003007593	A	20050201	BR 2003-7593	20030206
JP 2005517693	T	20050616	JP 2003-565454	20030206
CN 1630512	A	20050622	CN 2003-803580	20030206
NZ 533957	A	20060224	NZ 2003-533957	20030206
RU 2273473	C2	20060410	RU 2004-124065	20030206
AT 346591	T	20061215	AT 2003-737712	20030206
ZA 2004005556	A	20050810	ZA 2004-5556	20040713
NO 2004003716	A	20040906	NO 2004-3716	20040906
HK 1074581	A1	20061020	HK 2005-106918	20050811

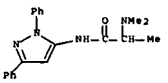
PRIORITY APPLN. INFO.:		
US 2002-355705P	P	20020207
WO 2003-US3837	W	20030206

OTHER SOURCE(S): MARPAT 139:185666

AB A pharmaceutical tablet is provide comprising a core and a coating adherent thereto, wherein (a) the core comprises solid particles of a water-soluble dye distributed in a matrix and (b) the coating comprises gellan gum. The tablet is suitable for peroral or intraoral administration, for example for delivery of a drug contained in the core of the tablet to a subject. The tablet has a speckled appearance that renders the tablet readily identifiable.

IT 20170-20-1, Difenamizole
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(active ingredients for coated pharmaceutical tablets with speckled appearance)

RN 20170-20-1 HCAPLUS
CN Propanamide, 2-(dimethylamino)-N-(1,3-diphenyl-1H-pyrazol-5-yl)- (9CI) (CA INDEX NAME)



L5 ANSWER 8 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:633447 HCAPLUS Full-text
DOCUMENT NUMBER: 139:185665
TITLE: Pharmaceutical dosage form for mucosal delivery
INVENTOR(S): Martino, Alice C.; Pierman, Steven A.; Noack, Robert M.; Britten, Nancy
PATENT ASSIGNEE(S): Pharmacia Corporation, USA
SOURCE: PCT Int. Appl., 34 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003066029	A2	20030814	WO 2003-US3836	20030206 <--
WO 2003066029	A3	20031016		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2474190	A1	20030814	CA 2003-2474190	20030206 <--
AU 2003215110	A1	20030902	AU 2003-215110	20030206 <--
US 2003235617	A1	20031225	US 2003-360167	20030206 <--
EP 1471890	A2	20041103	EP 2003-710927	20030206
EP 1471890	B1	20060927		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003007473	A	20041109	BR 2003-7473	20030206
CN 1627938	A	20050615	CN 2003-803419	20030206
JP 2005519924	T	20050707	JP 2003-565453	20030206
NZ 534340	A	20060428	NZ 2003-534340	20030206
AT 340565	T	20061015	AT 2003-710927	20030206
RU 2285520	C2	20061020	RU 2004-124057	20030206
ZA 2004005614	A	20050627	ZA 2004-5614	20040714
NO 2004003723	A	20040906	NO 2004-3723	20040906

PRIORITY APPLN. INFO.:		
US 2002-355703P	P	20020207
WO 2003-US3836	W	20030206

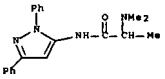
OTHER SOURCE(S): MARPAT 139:185665

AB A pharmaceutical tablet is provided comprising an intraorally disintegratable core and an excipient coating adherent thereto, wherein the coating comprises gellan gum. The tablet is suitable for intraoral administration, for example for delivery of a drug contained in the core of the tablet to a subject, at least in part by absorption of the drug via oral mucosa of the subject.

IT 20170-20-1, Difenamizole
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(active ingredients for coated sublingual tablets)

RN 20170-20-1 HCAPLUS
CN Propanamide, 2-(dimethylamino)-N-(1,3-diphenyl-1H-pyrazol-5-yl)- (9CI) (CA INDEX NAME)

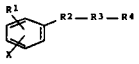


L5 ANSWER 9 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:570813 HCAPLUS Full-text
DOCUMENT NUMBER: 139:113668
TITLE: β-secretase inhibitors for use in treatment of diseases caused by deposits of β-amyloid peptides
INVENTOR(S): Dietrich, Axel; Nimz, Olaf; Rester, Ulrich; Fecke, Wolfgang; Haemmerle, Marcus; Baier, Friedrich
PATENT ASSIGNEE(S): The Genetics Company Inc., Switz.
SOURCE: PCT Int. Appl., 42 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003059346	A1	20030724	WO 2003-EP504	20030120 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2473441	A1	20030724	CA 2003-2473441	20030120 <--
AU 2003205630	A1	20030730	AU 2003-205630	20030120 <--
EP 1467729	A1	20041020	EP 2003-702474	20030120
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2005516967	T	20050609	JP 2003-559508	20030120
US 2005239899	A1	20051027	US 2005-502075	20050418

PRIORITY APPLN. INFO.:		
EP 2002-1339	A	20020118
EP 2002-12566	A	20020605
WO 2003-EP504	W	20030120

OTHER SOURCE(S): MARPAT 139:113668
GI

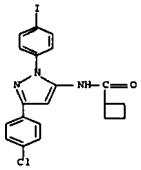


I

AB The invention relates to novel substituted halophenyl inhibitors of β-secretase (II, R1 = halo, hydroxy, cyano, trifluoromethyl, C1-4 substituted saturated or unsatd. alkyl, n = 0-4; X = halo, Me, trifluoromethyl; R2 = C1-8 alkyl containing at least one heteroatom and optionally unsatd.; R3 = aryl, carbocycle or heterocycle; R4 = R1 or a substituted aryl or heterocycle) and their use in treatment of diseases caused by deposits of β-amyloid, such as Alzheimer's disease. Thus, 7 compds. with IC50 10-170 μM in in vitro β-secretase assays are disclosed.

IT 562045-26-5
RL: BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(β-secretase inhibitors for use in treatment of diseases caused by deposits of β-amyloid peptides)

RN 562045-26-5 HCAPLUS
CN Cyclobutanecarboxamide, N-[3-(4-chlorophenyl)-1-(4-iodophenyl)-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

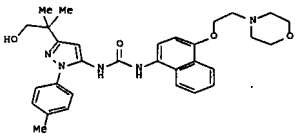


REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 10 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:150529 HCAPLUS Full-text
DOCUMENT NUMBER: 138:205052
TITLE: Preparation of 1-(pyrazol-3-yl)-3-(1-naphthyl)ureas as antiinflammatory agents
INVENTOR(S): Cirillo, Pier Francesco; Dinallo, Roger; Regan, John Robinson; Riska, Paul S.; Swinamer, Alan David; Tan, Zhulin; Walter, Brian Andrew
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE: U.S., 44 pp., Cont.-in-part of U.S. Ser. No. 879,776, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6525046	B1	20030225	US 2002-165372	20020607 <--
US 6319921	B1	20011120	US 2000-484638	20000118 <--
US 6333325	B1	20011225	US 2001-871559	20010531 <--
US 2002058678	A1	20020516	US 2001-879776	20010612 <--
US 6329415	B1	20011211	US 2001-891579	20010626 <--
US 2002065285	A1	20020530	US 2001-891820	20010626 <--
US 6506748	B2	20030114		
PRIORITY APPLN. INFO.:			US 2000-484638	A3 20000118
			US 2001-879776	B2 20010612
			US 1999-116400P	P 19990119
OTHER SOURCE(S):	MARPAT 138:205052			

GI



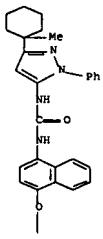
I

AB The title compds. Ar1NHC(:X)NHAr2LQ [Ar1 = pyrazolyl, pyrrolyl, imidazolyl, etc.; Ar2 = Ph, naphthyl, quinolyl, etc.; L = alkylene wherein one or more methylene groups are optionally replaced by O, N or S; Q = Ph, naphthyl, pyridyl, etc.; X = O, S], useful for treating diseases involving inflammation such as chronic inflammatory diseases, were prepared E.g., a multi-step synthesis of I, starting from Me 2,2-dimethyl-3-hydroxypropionate, was given. Representative title ureas showed IC50 of < 10 μM against TNF production in THP cells.

IT 285983-51-9P 285983-84-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 1-(pyrazol-3-yl)-3-(1-naphthyl)ureas as antiinflammatory agents)

RN 285983-51-9 HCAPLUS
CN Urea, N-[3-(1-methylcyclohexyl)-1-phenyl-1H-pyrazol-5-yl]-N'-[4-[2-(4-morpholinyl)ethoxy]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

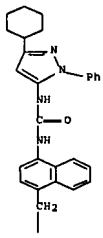
PAGE 1-A



PAGE 2-A

RN 285983-84-8 HCAPLUS
CN Urea, N-(3-cyclohexyl-1-phenyl-1H-pyrazol-5-yl)-N'-[4-[2-(4-morpholinyl)ethyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs hitstr 11-20

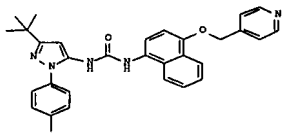
L5 ANSWER 11 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:57886 HCAPLUS Full-text
DOCUMENT NUMBER: 138:122641
TITLE: Method of treating cytokine mediated diseases using pyrazolylureas.
INVENTOR(S): Moss, Neil; Regan, John R.
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 84 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003005999	A2	20030123	WO 2002-US20649	20020701 <--
WO 2003005999	A3	20030417		
WO 2003005999	A8	20040422		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2453147	A1	20030123	CA 2002-2453147	20020701 <--
AU 2002316459	A1	20030129	AU 2002-316459	20020701 <--
US 2003130309	A1	20030710	US 2002-187942	20020701 <--
US 6916814	B2	20050712		
EP 1408950	A2	20040421	EP 2002-746764	20020701
EP 1408950	B1	20070425		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004536845	T	20041209	JP 2003-511806	20020701
EP 1709965	A2	20061011	EP 2006-112554	20020701
EP 1709965	A3	20061227		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				
US 2004152725	A1	20040805	US 2004-761913	20040120
PRIORITY APPLN. INFO.:			US 2001-304511P	P 20010711

	EP 2002-746764	A3	20020701
	US 2002-187942	A3	20020701
	WO 2002-US20649	W	20020701

OTHER SOURCE(S): MARPAT 138:122641

GI



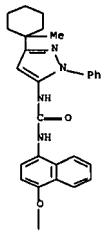
I

AB A method of treating lung inflammation, endometriosis, behcet's disease, uveitis, ankylosing spondylitis, pancreatitis, cancer, percutaneous transluminal coronary angioplasty, alzheimer's disease, traumatic arthritis, sepsis, chronic obstructive pulmonary disease, and congestive heart failure comprises administration of Ar1NHC(:X)NHAr2LQ [Ar1 = (substituted) pyrrolyl, pyrrolidinyl, pyrazolyl, imidazolyl, oxazolyl, thiazolyl, furyl, thienyl; Ar2 = (substituted) Ph, naphthyl, quinolinyl, isoquinolinyl, tetrahydronaphthyl, tetrahydroisoquinolinyl, benzimidazolyl, benzofuryl, indanyl, indolyl, etc.; L = (O-, S-, or N-interrupted) (unsatd.) (substituted) alkylene; Q = (substituted) Ph, naphthyl, pyridyl, pyrimidinyl, imidazolyl, tetrahydropyranyl, tetrahydrofuryl, dioxanyl, alkoxy, amino, etc.; X = O, S]. Thus, 5-amino-3-tert-butyl-1-(4-methylphenyl)pyrazole was stirred with COCl2 and NaHCO3 in PhMe/CH2Cl2 at 0-5° for 15 min. The organic residue was stirred overnight with 1-amino-4-(4-pyridinylmethoxy)naphthalene dihydrochloride (preparation given) and diisopropylethylamine in THF to give title compound (I). Representative title compds. inhibited TNF production in THP cells with IC50<10 μM.

IT 285983-51-9P 285983-84-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(method of treating cytokine mediated diseases using pyrazolylureas)

RN 285983-51-9 HCAPLUS
CN Urea, N-[3-(1-methylcyclohexyl)-1-phenyl-1H-pyrazol-5-yl]-N'-[4-[2-(4-morpholinyl)ethoxy]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

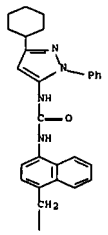
PAGE 1-A



PAGE 2-A

RN 285983-84-8 HCAPLUS
CN Urea, N-(3-cyclohexyl-1-phenyl-1H-pyrazol-5-yl)-N'-[4-[2-(4-morpholinyl)ethyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

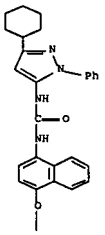
PAGE 1-A



PAGE 2-A

IT 285983-96-2
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(method of treating cytokine mediated diseases using pyrazolylureas)
RN 285983-96-2 HCAPLUS
CN Urea, N-(3-cyclohexyl-1-phenyl-1H-pyrazol-5-yl)-N'-[4-[2-(4-morpholinyl)ethoxy]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

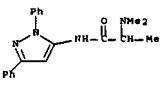
PAGE 1-A



PAGE 2-A

L5 ANSWER 12 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:49279 HCAPLUS Full-text
DOCUMENT NUMBER: 139:159420
TITLE: Discrimination and selection of new potential

antibacterial compounds using simple topological descriptors
AUTHOR(S): Murcia-Soler, Miguel; Perez-Gimenez, Facundo; Garcia-March, Francisco J.; Salabert-Salvador, M. Teresa; Diaz-Villanueva, Wladimiro; Medina-Casamayor, Piedad
CORPORATE SOURCE: Faculty of Pharmacy, Department of Physical Chemistry, Universitat de Valencia, Valencia, Spain
SOURCE: Journal of Molecular Graphics & Modelling (2003), 21(5), 375-390
CODEN: JMGMPI; ISSN: 1093-3263
PUBLISHER: Elsevier Science Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The aim of the work was to discriminate between antibacterial and non-antibacterial drugs by topol. methods and to select new potential antibacterial agents from among new structures. The method used for antibacterial activity selection was a linear discriminant anal. (LDA). It is possible to obtain a QSAR interpretation of the information contained in the discriminant function. We make use of the pharmacol. distribution diagrams (PDDs) as a visualizing technique for the identification and selection of new antibacterial agents.
IT 20170-20-1, Difenamizole
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(discrimination and selection of new potential antibacterial compds. using simple topol. descriptors)
RN 20170-20-1 HCAPLUS
CN Propanamide, 2-(dimethylamino)-N-(1,3-diphenyl-1H-pyrazol-5-yl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 13 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:942809 HCAPLUS Full-text
DOCUMENT NUMBER: 138:24709
TITLE: Preparation of pyrazole compounds and bis pyrazole-1H-pyrazole intermediates as antiinflammatory agents
INVENTOR(S): Kapadia, Suresh R.; Song, Jinhua J.; Yee, Nathan K.
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE: U.S., 37 pp., Cont.-in-part of U.S. 6,372,773.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6492529	B1	20021210	US 2002-67492	20020205 <--
US 6319921	B1	20011120	US 2000-484638	20000118 <--
US 6333325	B1	20011225	US 2001-871559	20010531 <--

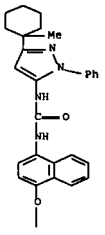
US 6329415	B1	20011211	US 2001-891579	20010626 <--
US 2002065285	A1	20020530	US 2001-891820	20010626 <--
US 6506748	B2	20030114		
US 6372773	B1	20020416	US 2001-920899	20010802 <--

PRIORITY APPLN. INFO.:
US 2001-920899 A3 20000118
US 2001-920899 A2 20010802
US 1999-116400P P 19990119
US 2001-891579 A3 20010626
OTHER SOURCE(S): CASREACT 138:24709; MARPAT 138:24709
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Pyrazole compds., e.g. I, as well as bis pyrazole-1H-pyrazole intermediate compds. e.g. II, were prepared The compds. are useful in pharmaceutic compns. for treating diseases or pathol. conditions involving inflammation such as chronic inflammatory diseases. All prepared compds. had IC50 < 10 mM for inhibition of TNFα in lipopolysaccharide stimulated THP cells.
IT 285983-51-9P 285983-84-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazole compds. and bis pyrazole-1H-pyrazole intermediates as antiinflammatory agents)
RN 285983-51-9 HCAPLUS
CN Urea, N-[3-(1-methylcyclohexyl)-1-phenyl-1H-pyrazol-5-yl]-N'-[4-[2-(4-morpholinyl)ethoxy]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

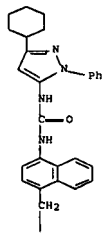
PAGE 1-A



PAGE 2-A

RN 285983-84-8 HCAPLUS
CN Urea, N-(3-cyclohexyl-1-phenyl-1H-pyrazol-5-yl)-N'-[4-[2-(4-morpholinyl)ethyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 14 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:595343 HCAPLUS Full-text
DOCUMENT NUMBER: 137:150228
TITLE: Antiinflammatory compositions and methods for therapy through enhanced tissue regeneration
INVENTOR(S): Uhrich, Kathryn E.; Macedo, Braz
PATENT ASSIGNEE(S): Rutgers, The State University of New Jersey, USA
SOURCE: U.S. Pat. Appl. Publ., 17 pp.

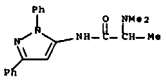
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002106345	A1	20020808	US 2000-732516	20001207 <--
US 6685928	B2	20040203		
AU 2006201924	A1	20060601	AU 2006-201924	20060509
US 2007014832	A1	20070118	US 2006-524664	20060921
PRIORITY APPLN. INFO.:			US 1999-304190P P	19991207
			US 1999-455861 A	19991207
			AU 2001-19565 A3	20001207
			US 2000-732516 A1	20001207
			WO 2000-US33378 A1	20001207
			US 2003-368288 B1	20030218

AB The invention provides methods of promoting healing through enhanced regeneration of tissue (e.g. hard tissue or soft tissue) by contacting the tissue or the surrounding tissue with an antiinflammatory agent, preferably in a controlled-release form, e.g. by dispersing the agent through a polymer matrix, appending the agent to a polymer backbone, or incorporating the agent directly into a biodegradable polymer backbone. These methods are useful in a variety of dental and orthopedic applications. Expts. are presented which demonstrate that implantation of a film comprising an aromatic polyanhydride that hydrolyzes to form a therapeutically useful salicylate resulted in less swelling in tissues adjacent to the film and a decrease in the d. of inflammatory cells as compared to other polyanhydride films. Preparation of e.g. poly[1,6-bis(o-carboxyphenoxy) hexane] is described.

IT 20170-20-1, Difenamizole
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(antiinflammatory compns. and methods for therapy through enhanced tissue regeneration)

RN 20170-20-1 HCAPLUS
CN Propanamide, 2-(dimethylamino)-N-(1,3-diphenyl-1H-pyrazol-5-yl)- (9CI) (CA INDEX NAME)

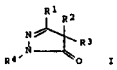


L5 ANSWER 15 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:483069 HCAPLUS Full-text
DOCUMENT NUMBER: 137:47195
TITLE: Preparation of pyrazole derivs. as antibacterial agents
INVENTOR(S): Hirth, Bradford H.; Janjigian, Andrew; Vinick, Fred
PATENT ASSIGNEE(S): Genzyme Corporation, USA
SOURCE: U.S., 18 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

US 6410533	B1	20020625	US 2000-502101	20000210 <--
PRIORITY APPLN. INFO.:			US 2000-502101	20000210
OTHER SOURCE(S):	MARPAT 137:47195			

GI



AB The compound of the formula I [R1 = substituted aryl, (un)substituted arylalkyl, alkyl, perfluoroalkyl, heteroaryl, carboxy, carboxamido, amino or alkoxycarbonyl or heteroaryl; R2 and R3 are each, independently = H, (un)substituted, linear, cyclic or branched alkyl, aminoalkyl, arylalkyl, heteroarylalkyl, heteroarylcarbonyl, alkylidene group, or together form :N-OH; R4 = (un)substituted Ph group] were prepared as antibacterial agents. Thus, a solution of Et benzoylacetate, 3,5-dichlorophenylhydrazine hydrochloride and p-toluenesulfonic acid monohydrate in ethanol was heated at reflux for 24 h. to give 0.174 g of the 2-(3,5-dichlorophenyl)-5-phenyl- 2,4-dihydro-pyrazol-3-one, which showed MIC (minimal inhibitory concentration) = 0.122 μg/mL for Streptococcus aureus bacteria.

IT 438242-75-2P 438242-76-3P 438242-77-4P
438242-78-5P 438242-79-6P 438242-80-9P
438242-81-0P 438242-82-1P 438242-88-7P
438242-92-3P 438243-00-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazole derivs. as antibacterial agents)

RN 438242-75-2 HCAPLUS
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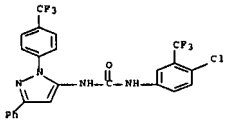
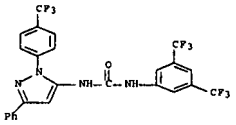
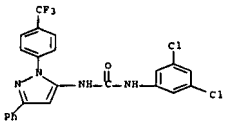


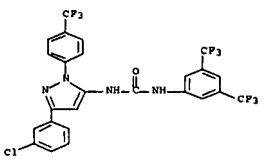
RN 438242-76-3 HCAPLUS
CN Urea, N-[3,5-bis(trifluoromethyl)phenyl]-N'-[3-phenyl-1-[4-(trifluoromethyl)phenyl]-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)



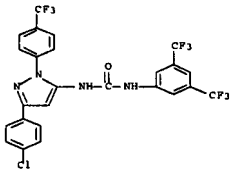
RN 438242-77-4 HCAPLUS
CN Urea, N-(3,5-dichlorophenyl)-N'-[3-phenyl-1-[4-(trifluoromethyl)phenyl]-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)



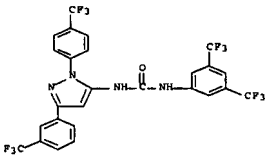
RN 438242-78-5 HCAPLUS
CN Urea, N-[3,5-bis(trifluoromethyl)phenyl]-N'-[3-(3-chlorophenyl)-1-[4-(trifluoromethyl)phenyl]-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)



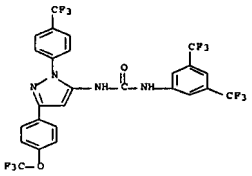
RN 438242-79-6 HCAPLUS
CN Urea, N-[3,5-bis(trifluoromethyl)phenyl]-N'-[3-(4-chlorophenyl)-1-[4-(trifluoromethyl)phenyl]-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)



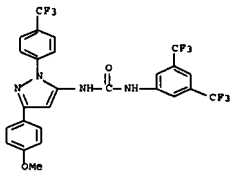
RN 438242-80-9 HCAPLUS
CN Urea, N-[3,5-bis(trifluoromethyl)phenyl]-N'-[3-[3-(trifluoromethyl)phenyl]-1-[4-(trifluoromethyl)phenyl]-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)



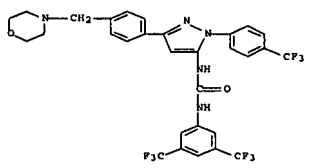
RN 438242-81-0 HCAPLUS
CN Urea, N-[3,5-bis(trifluoromethyl)phenyl]-N'-[3-[4-(trifluoromethoxy)phenyl]-1-[4-(trifluoromethyl)phenyl]-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)



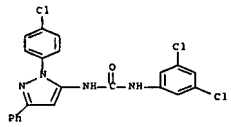
RN 438242-82-1 HCAPLUS
CN Urea, N-[3,5-bis(trifluoromethyl)phenyl]-N'-[3-(4-methoxyphenyl)-1-[4-(trifluoromethyl)phenyl]-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)



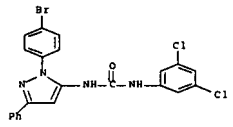
RN 438242-88-7 HCAPLUS
CN Urea, N-[3,5-bis(trifluoromethyl)phenyl]-N'-[3-[4-(4-morpholinylmethyl)phenyl]-1-[4-(trifluoromethyl)phenyl]-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)



RN 438242-92-3 HCAPLUS
CN Urea, N-[1-(4-chlorophenyl)-3-phenyl-1H-pyrazol-5-yl]-N'-(3,5-dichlorophenyl)- (9CI) (CA INDEX NAME)



RN 438243-08-4 HCAPLUS
CN Urea, N-[1-(4-bromophenyl)-3-phenyl-1H-pyrazol-5-yl]-N'-(3,5-dichlorophenyl)- (9CI) (CA INDEX NAME)



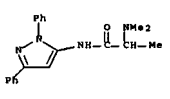
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 16 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:426876 HCAPLUS Full-text
DOCUMENT NUMBER: 137:149790
TITLE: Structure-Based Classification of Antibacterial Activity
AUTHOR(S): Cronin, Mark T. D.; Aptula, Aynur O.; Dearden, John C.; Duffy, Judith C.; Netzeva, Tatiana I.; Patel, Hiren; Rowe, Philip H.; Schultz, T. Wayne; Worth, Andrew P.; Voutzoulidis, Konstantinos; Schueuermann, Gerrit
CORPORATE SOURCE: School of Pharmacy and Chemistry, Liverpool John Moores University, Liverpool, L3 3AF, UK
SOURCE: Journal of Chemical Information and Computer Sciences (2002), 42(4), 869-878
CODEN: JCISD8; ISSN: 0095-2338
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The aim of this study was to develop a simple quant. structure-activity relation (QSAR) for the classification and prediction of antibacterial activity, to enable in silico screening. To this end a database of 661 compds., classified according to whether they had antibacterial activity, and for which a total of 167 physicochem. and structural descriptors were calculated, was analyzed. To identify descriptors that allowed separation of the two classes (i.e. those compds. with and without antibacterial activity), anal. of variance was utilized and models were developed using linear discriminant and binary logistic regression analyses. Model predictivity was assessed and validated by the random removal of 30% of the compds. to form a test set, for which predictions were made from the model. The results of the analyses indicated that six descriptors, accounting for hydrophobicity and inter- and intramol. hydrogen bonding, provided excellent separation of the data. Logistic regression anal. was shown to model the data slightly more accurately than discriminant anal.

IT 20170-20-1
RL: PAC (Pharmacological activity); BIOL (Biological study)
(structure-based classification of antibacterial activity)

RN 20170-20-1 HCAPLUS
CN Propanamide, 2-(dimethylamino)-N-(1,3-diphenyl-1H-pyrazol-5-yl)- (9CI) (CA INDEX NAME)



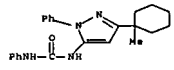
REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 17 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:392357 HCAPLUS Full-text
DOCUMENT NUMBER: 137:119059
TITLE: Pyrazole Urea-Based Inhibitors of p38 MAP Kinase: From Lead Compound to Clinical Candidate
AUTHOR(S): Regan, John; Breitfelder, Steffen; Cirillo, Pier; Gilmore, Thomas; Graham, Anne G.; Hickey, Eugene; Klaus, Bernhard; Madwed, Jeffrey; Moriak, Monica; Moss, Neil; Pargellis, Chris; Pav, Sue; Proto, Alfred; Swinamer, Alan; Tong, Liang; Torcellini, Carol
CORPORATE SOURCE: Research and Development Center, Department of Medicinal Chemistry, Boehringer Ingelheim Pharmaceuticals, Ridgefield, CT, 06877, USA
SOURCE: Journal of Medicinal Chemistry (2002), 45(14), 2994-3008
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:119059

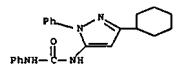
AB We report on a series of N-pyrazole, N'-aryl ureas and their mode of binding to p38 mitogen activated protein kinase. Importantly, a key binding domain that is distinct from the ATP (ATP) binding site is exposed when the conserved activation loop, consisting in part of Asp168-Phe169-Gly170, adopts a conformation permitting lipophilic and hydrogen bonding interactions between this class of inhibitors and the protein. We describe the correlation of the structure-activity relationships and crystallog. structures of these inhibitors with p38. In addition, we incorporated another binding pharmacophore that forms a hydrogen bond at the ATP binding site. This modification affords significant improvements in binding, cellular, and in vivo potencies resulting in the selection of Compound 45 (BIRB 796) as a clin. candidate for the treatment of inflammatory diseases.

IT 223724-97-8P 443913-00-6P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(structure activity relationships of N-pyrazole, N'-aryl ureas and their mode of binding to p38 mitogen activated protein kinase)

RN 223724-97-8 HCAPLUS
CN Urea, N-[3-(1-methylcyclohexyl)-1-phenyl-1H-pyrazol-5-yl]-N'-phenyl- (9CI) (CA INDEX NAME)



RN 443913-00-6 HCAPLUS
CN Urea, N-(3-cyclohexyl-1-phenyl-1H-pyrazol-5-yl)-N'-phenyl- (9CI) (CA INDEX NAME)



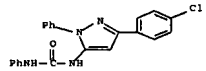
REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 18 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:294376 HCAPLUS Full-text
DOCUMENT NUMBER: 137:41265
TITLE: Molecular docking and high-throughput screening for novel inhibitors of protein tyrosine phosphatase-1B
AUTHOR(S): Doman, Thompson N.; McGovern, Susan L.; Witherbee, Bryan J.; Kasten, Thomas P.; Kurumbail, Ravi; Stallings, William C.; Connolly, Daniel T.; Shoichet, Brian K.
CORPORATE SOURCE: Pharmacia Corporation, Skokie, IL, 60077, USA
SOURCE: Journal of Medicinal Chemistry (2002), 45(11), 2213-2221
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB High-throughput screening (HTS) of compound libraries is used to discover novel leads for drug development. When a structure is available for the target, computer-based screening using mol. docking may also be considered. The two techniques have rarely been used together on the same target. The opportunity to do so presented itself in a project to discover novel inhibitors for the enzyme protein tyrosine phosphatase-1B (PTP1B), a tyrosine phosphatase that has been implicated as a key target for type II diabetes. A corporate library of approx. 400 000 compds. was screened using high-throughput exptl. techniques for compds. that inhibited PTP1B. Concurrently, mol. docking was used to screen approx. 235 000 com. available compds. against the X-ray crystallog. structure of PTP1B, and 365 high-scoring mols. were tested as inhibitors of the enzyme. Of approx. 400 000 mols. tested in the high-throughput exptl. assay, 85 (0.021%) inhibited the enzyme with IC50 values less than 100 μM; the most active had an IC50 value of 4.2 μM. Of the 365 mols. suggested by mol. docking, 127 (34.8%) inhibited PTP1B with IC50 values less than 100 μM; the most active of these had an IC50 of 1.7 μM. Structure-based docking therefore enriched the hit rate by 1700-fold over random screening. The hits from both the high-throughput and docking screens were dissimilar from phosphotyrosine, the canonical substrate group for PTP1B; the two hit lists were also very different from each other. Surprisingly, the docking hits were judged to be more druglike than the HTS hits. The diversity of both hit lists and their dissimilarity from each other suggest that docking and HTS may be complementary techniques for lead discovery.

IT 438046-45-8
RL: PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study)
(mol. docking and high-throughput screening for novel inhibitors of protein tyrosine phosphatase-1B)

RN 438046-45-8 HCAPLUS
CN Urea, N-[3-(4-chlorophenyl)-1-phenyl-1H-pyrazol-5-yl]-N'-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

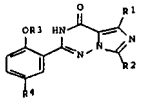
L5 ANSWER 19 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:657494 HCAPLUS Full-text
DOCUMENT NUMBER: 135:211060
TITLE: Preparation of 2-phenylimidazotriazinones as cGMP-metabolizing phosphodiesterase inhibitors
INVENTOR(S): Niewoehner, Ulrich; Es-Sayed, Mazen; Lampe, Thomas; Haning, Helmut; Schmidt, Gunther; Schlemmer, Karl-Heinz; Bischoff, Erwin; Dembowsky, Klaus; Perzborn, Elisabeth
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Ger. Offen., 154 pp.
CODEN: GMXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10010067	A1	20010906	DE 2000-10010067	20000302 <--
CA 2401834	A1	20010907	CA 2001-2401834	20010220 <--
WO 2001064677	A1	20010907	WO 2001-EP1871	20010220 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1280805	A1	20030205	EP 2001-911663	20010220 <--
EP 1280805	B1	20050209		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2001008853	A	20030429	BR 2001-8853	20010220 <--
JP 2003525293	T	20030826	JP 2001-564174	20010220 <--
AT 288916	T	20050215	AT 2001-911663	20010220
PT 1280805	T	20050630	PT 2001-911663	20010220
ES 2236190	T3	20050716	ES 2001-1911663	20010220
ZA 2002006217	A	20030805	ZA 2002-6217	20020805 <--
IN 2002MN01095	A	20040529	IN 2002-MN1095	20020813
US 2004097498	A1	20040520	US 2003-220560	20030206
US 6878708	B2	20050412		
HK 1055423	A1	20060825	HK 2003-106960	20030926
US 2005267112	A1	20051201	US 2005-30605	20050105
US 7098207	B2	20060829		

PRIORITY APPLN. INFO.: DE 2000-10010067 A 20000302
WO 2001-EP1871 W 20010220
US 2003-220560 A1 20030206

OTHER SOURCE(S): MARPAT 135:211060

GI

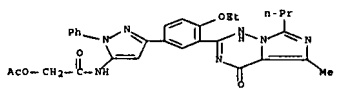


I

AB Title compds. [I; R1 = alkyl; R2 = cycloalkyl, alkyl; R3 = alkyl; R4 = NHSO2R5, N(SO2R6)SO2R7, etc.; R5, R6, R7 = (substituted) vinyl, alkyl, aryl; or R5 = quinolyl, (substituted) heteroaryl, etc.], were prepared as phosphodiesterase I and phosphodiesterase V inhibitors (no data). Thus, 2-(5-amino-2-ethoxyphenyl)-5-methyl-7-cyclopentyl-3H-imidazo[5,1- f][1,2,4]triazin-4-one (preparation given) in THF was treated at 5° with 4-morpholinocarbonyl chloride in THF followed by stirring overnight at room temperature to give 98% 2-[2-ethoxy-5-(4-morpholinocarbonylamino)phenyl]-5- methyl-7-cyclopentyl-3H-imidazo[5,1-f][1,2,4]triazin-4-one.

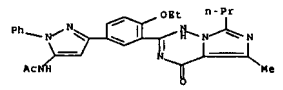
IT 358390-19-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of phenylimidazotriazinones as cGMP-metabolizing phosphodiesterase inhibitors)

RN 358390-19-9 HCAPLUS
CN Acetamide, 2-(acetyloxy)-N-[3-[3-(1,4-dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]-1-phenyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

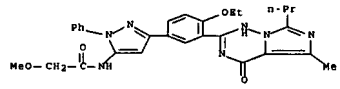


IT 358390-14-4P 358390-17-7P 358390-18-8P 358390-20-2P 358390-21-3P 358390-26-8P 358390-27-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of phenylimidazotriazinones as cGMP-metabolizing phosphodiesterase inhibitors)

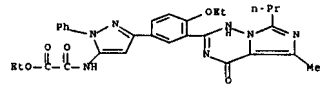
RN 358390-14-4 HCAPLUS
CN Acetamide, N-[3-[3-(1,4-dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]-1-phenyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)



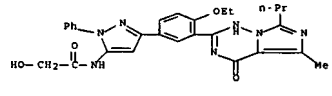
RN 358390-17-7 HCAPLUS
CN Acetamide, N-[3-[3-(1,4-dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]-1-phenyl-1H-pyrazol-5-yl]-2-methoxy- (9CI) (CA INDEX NAME)



RN 358390-18-8 HCAPLUS
CN Acetic acid, [[3-[3-(1,4-dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]-1-phenyl-1H-pyrazol-5-yl]amino]oxo-, ethyl ester (9CI) (CA INDEX NAME)

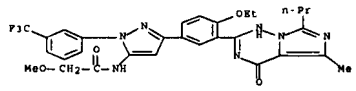


RN 358390-20-2 HCAPLUS
CN Acetamide, N-[3-[3-(1,4-dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]-1-phenyl-1H-pyrazol-5-yl]-2-hydroxy- (9CI) (CA INDEX NAME)

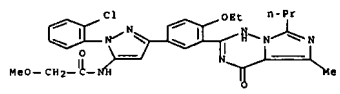


RN 358390-21-3 HCAPLUS
CN Acetamide, N-[3-[3-(1,4-dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]-1-[3-(trifluoromethyl)phenyl]-1H-

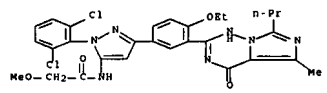
pyrazol-5-yl]-2-methoxy- (9CI) (CA INDEX NAME)



RN 358390-26-8 HCAPLUS
CN Acetamide, N-[1-(2-chlorophenyl)-3-[3-(1,4-dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]-1H-pyrazol-5-yl]-2-methoxy- (9CI) (CA INDEX NAME)



RN 358390-27-9 HCAPLUS
CN Acetamide, N-[1-(2,6-dichlorophenyl)-3-[3-(1,4-dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]-1H-pyrazol-5-yl]-2-methoxy- (9CI) (CA INDEX NAME)

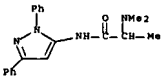


L5 ANSWER 20 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:434854 HCAPLUS Full-text
DOCUMENT NUMBER: 135:51045
TITLE: Therapeutic compositions containing anti-inflammatory agents and biodegradable polyanhydrides
INVENTOR(S): Uhrich, Kathryn; Macedo, Braz
PATENT ASSIGNEE(S): Rutgers, the State University of New Jersey, USA; University of Medicine and Dentistry
SOURCE: PCT Int. Appl., 40 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 2001041753	A2	20010614	WO 2000-US33378	20001207 <--
WO 2001041753	A3	20020912		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2393676	A1	20010614	CA 2000-2393676	20001207 <--
EP 1261347	A1	20021204	EP 2000-982544	20001207 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003528044	T	20030924	JP 2001-543098	20001207 <--
US 2004038948	A1	20040226	US 2003-368288	20030218
AU 2006201924	A1	20060601	AU 2006-201924	20060509
US 2007014832	A1	20070118	US 2006-524664	20060921
PRIORITY APPLN. INFO.:			US 1999-455861	A 19991207
			US 1999-304190P	P 19991207
			AU 2001-19565	A3 20001207
			US 2000-732516	A1 20001207
			WO 2000-US33378	W 20001207
			US 2002-165220	B1 20020607
			US 2003-368288	B1 20030218

AB Methods of promoting healing through enhanced regeneration of tissue (e.g. hard tissue or soft tissue) by contacting the tissue or the surrounding tissue with an antiinflammatory agent are useful in a variety of dental and orthopedic applications. Thus, poly[1,6-bis(o-carboxyphenoxy)hexane] was prepared in a series of steps by the treatment of salicylic acid with 1,6-dibromohexane, and polymerization of the resulting 1,6-bis(o-carboxyphenoxy)hexane. The polymer was characterized by glass transition temperature measurements and then subjected to compression molding.
IT 20170-20-1, Difenamizole
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(therapeutic compns. containing antiinflammatory agents and biodegradable polyanhydrides)
RN 20170-20-1 HCAPLUS
CN Propanamide, 2-(dimethylamino)-N-(1,3-diphenyl-1H-pyrazol-5-yl)- (9CI) (CA INDEX NAME)

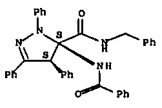


=> d ibib abs hitstr 21-30

L5 ANSWER 21 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:223058 HCAPLUS Full-text
DOCUMENT NUMBER: 135:33441
TITLE: Reaction of benzonitrilium N-phenylimide with (Z)-4-arylmethyleneimidazol-5(4H)-ones
AUTHOR(S): Abdallah, M. A.; Zayed, M. E.; Shawali, A. S.
CORPORATE SOURCE: Department of Chemistry, Faculty of Science,

University of Cairo, Giza, Egypt
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (2001), 40B(3), 187-190
CODEN: IJSBDB; ISSN: 0376-4699
PUBLISHER: National Institute of Science Communication, CSIR
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:33441
AB The title reaction, when carried out in chloroform in the presence of triethylamine, yields the spirocycloadducts which upon treatment with a base affords 1,3,4-triaryl-5-pyrazolecarboxamide.
IT 344346-87-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(reaction of benzonitrilium N-phenylimide with (Z)-4-arylmethyleneimidazol-5(4H)-ones)
RN 344346-87-8 HCAPLUS
CN 1H-Pyrazole-5-carboxamide, 5-(benzoylamino)-4,5-dihydro-1,3,4-triphenyl-N-(phenylmethyl)-, (4R,5R)-rel- (9CI) (CA INDEX NAME)

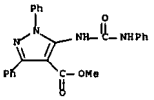
Relative stereochemistry.



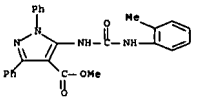
REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 22 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:825371 HCAPLUS Full-text
DOCUMENT NUMBER: 134:131489
TITLE: A convenient synthesis of pyrazolo[3,4-d]pyrimidine-4,6-dione and pyrazolo[4,3-d]pyrimidine-5,7-dione derivatives
AUTHOR(S): Haddad, M. El; Soukri, M.; Lazar, S.; Bennamara, A.; Guillaumet, G.; Akssira, M.
CORPORATE SOURCE: Laboratoire de Chimie Bioorganique et Analytique, FST - Universite Hassan II - Mohammedia, Mohammedia, Morocco
SOURCE: Journal of Heterocyclic Chemistry (2000), 37(5), 1247-1252
CODEN: JHTCAD; ISSN: 0022-152X
PUBLISHER: HeteroCorporation
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:131489
AB Pyrazolo[3,4-d]pyrimidine-4,6-diones and pyrazolo[4,3-d]pyrimidine-5,7- diones were synthesized by Curtius rearrangement of 3,4- pyrazoledicarboxylic acid monoesters followed by heterocyclization via urea derivs. under alkaline conditions.
IT 321850-61-7P 321850-62-8P 321850-63-9P 321850-64-0P 321850-66-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrazolopyrimidinediones)

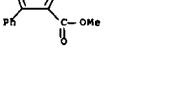
RN 321850-61-7 HCAPLUS
CN 1H-Pyrazole-4-carboxylic acid, 1,3-diphenyl-5-[[(phenylamino)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



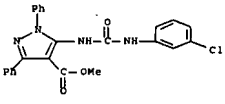
RN 321850-62-8 HCAPLUS
CN 1H-Pyrazole-4-carboxylic acid, 5-[[[(2-methylphenyl)amino]carbonyl]amino]-1,3-diphenyl-, methyl ester (9CI) (CA INDEX NAME)



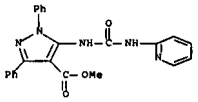
RN 321850-63-9 HCAPLUS
CN 1H-Pyrazole-4-carboxylic acid, 5-[[[(2-ethylphenyl)amino]carbonyl]amino]-1,3-diphenyl-, methyl ester (9CI) (CA INDEX NAME)



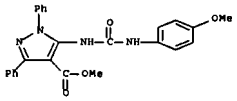
RN 321850-64-0 HCAPLUS
CN 1H-Pyrazole-4-carboxylic acid, 5-[[[(3-chlorophenyl)amino]carbonyl]amino]-1,3-diphenyl-, methyl ester (9CI) (CA INDEX NAME)



RN 321850-66-2 HCAPLUS
CN 1H-Pyrazole-4-carboxylic acid, 1,3-diphenyl-5-[[(2-pyridinylamino)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



IT 321850-66-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of pyrazolopyrimidinediones)
RN 321850-65-1 HCAPLUS
CN 1H-Pyrazole-4-carboxylic acid, 5-[[[(4-methoxyphenyl)amino]carbonyl]amino]-1,3-diphenyl-, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 23 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:513688 HCAPLUS Full-text
DOCUMENT NUMBER: 133:120325
TITLE: Preparation of aromatic heterocyclic ureas as antiinflammatory agents
INVENTOR(S): Cirillo, Pier F.; Gilmore, Thomas A.; Hickey, Eugene R.; Regan, John R.; Zhang, Lin-Hua
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 96 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000043384	A1	20000727	WO 1999-US29165	19991209 <--
W: AE, AU, BG, BR, BY, CA, CN, CZ, EE, HR, HU, ID, IL, IN, JP, KR, KZ, LT, LV, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, UA, UZ, VN, YU, ZA				

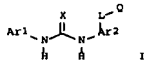
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE

CA 2352524	A1	20000727	CA 1999-2352524	19991209 <--
EP 1147104	A1	20011024	EP 1999-960668	19991209 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 9916930	A	20011030	BR 1999-16930	19991209 <--
HU 200201406	A2	20020828	HU 2002-1406	19991209 <--
HU 200201406	A3	20031128		
EE 200100376	A	20021015	EE 2001-376	19991209 <--
EE 4527	B1	20050815		
JP 2003535023	T	20031125	JP 2000-594800	19991209 <--
JP 3793694	B2	20060705		
RU 2220142	C2	20031227	RU 2001-122111	19991209 <--
AU 770581	B2	20040226	AU 2000-17522	19991209
NZ 513525	A	20040528	NZ 1999-513525	19991209
TR 200102072	T2	20041221	TR 2001-200102072	19991209
TW 546297	B	20030811	TW 2000-89100638	20000117 <--
US 6333325	B1	20011225	US 2001-871559	20010531 <--
IN 2001MN00642	A	20050304	IN 2001-MN642	20010604
ZA 2001004656	A	20030210	ZA 2001-4656	20010607 <--
US 6329415	B1	20011211	US 2001-891579	20010626 <--
US 2002065285	A1	20020530	US 2001-891820	20010626 <--
US 6506748	B2	20030114		
BG 105653	A	20020131	BG 2001-105653	20010627 <--
BG 64971	B1	20061130		
HR 2001000516	A1	20020831	HR 2001-516	20010710 <--
NO 2001003559	A	20010718	NO 2001-3559	20010718 <--

PRIORITY APPLN. INFO.:

US 1999-116400P	P	19990119
WO 1999-US29165	W	19991209
US 2000-484638	A1	20000118

OTHER SOURCE(S): MARPAT 133:120325
GI



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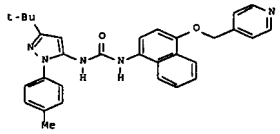

II

AB The title compds. [I; Ar1 = (un)substituted pyrrole, pyrrolidine, pyrazole, etc.; Ar2 = (un)substituted Ph, naphthyl, quinoline, etc.; L = (un)saturated (un)substituted carbon chain wherein one or more methylene groups are optionally replaced by O, N, or S; Q = (un)substituted Ph, naphthyl, pyridinyl, etc.], useful in pharmaceutic compns. for

treating diseases or pathol. conditions involving inflammation such as chronic inflammatory diseases, were prepared E.g., a multi-step synthesis of the urea II was given. Representative compds. I were evaluated and showed IC50 of < 10 μM against TNF production in THP cells.

IT 285983-51-9P 285983-84-8P 285983-96-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aromatic heterocyclic ureas as antiinflammatory agents)
RN 285983-51-9 HCAPLUS
CN Urea, N-[3-(1-methylcyclohexyl)-1-phenyl-1H-pyrazol-5-yl]-N'-[4-[2-(4-morpholinyl)ethoxy]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

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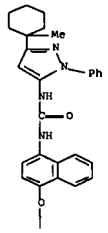
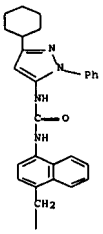


PAGE 2-A

RN 285983-84-8 HCAPLUS
CN Urea, N-(3-cyclohexyl-1-phenyl-1H-pyrazol-5-yl)-N'-[4-[2-(4-morpholinyl)ethyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

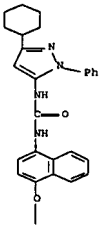
PAGE 1-A



PAGE 2-A

RN 285983-96-2 HCAPLUS
CN Urea, N-(3-cyclohexyl-1-phenyl-1H-pyrazol-5-yl)-N'-[4-[2-(4-morpholinyl)ethoxy]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



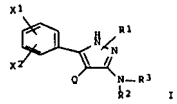
PAGE 2-A

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 24 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:457057 HCAPLUS Full-text
DOCUMENT NUMBER: 133:58801
TITLE: Preparation of aminopyrazole derivatives as p38 mitogen-activated protein (p38MAP) kinase inhibitors
INVENTOR(S): Minami, Nobuyoshi; Sato, Michitaka; Hasumi, Koichi; Yamamoto, Norio; Keino, Katsuyuki; Matsui, Teruaki; Kanada, Arihiro; Ohta, Shuji; Saito, Takahisa; Sato, Shuichiro; Asagarasu, Akira; Doi, Satoshi; Kobayashi, Motohiro; Sato, Jun; Asano, Hajime
PATENT ASSIGNEE(S): Teikoku Hormone Mfg. Co., Ltd., Japan
SOURCE: PCT Int. Appl., 111 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000039116	A1	20000706	WO 1999-JP7186	19991221 <--
W: AU, CA, CN, JP, KR, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2356263	A1	20000706	CA 1999-2356263	19991221 <--
EP 1142890	A1	20011010	EP 1999-959946	19991221 <--
EP 1142890	B1	20050803		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
AU 765492	B2	20030918	AU 2000-16911	19991221 <--
AT 301116	T	20050815	AT 1999-959946	19991221
ES 2244231	T3	20051201	ES 1999-959946	19991221
US 6511997	B1	20030128	US 2001-869051	20010622 <--
PRIORITY APPLN. INFO.:			JP 1998-371094 A	19981225
			WO 1999-JP7186 W	19991221
OTHER SOURCE(S):	MARPAT 133:58801			

GI



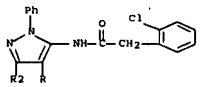
I

AB Aminopyrazole derivs. represented by general formula (I) or salts thereof [wherein X1 and X2 are each hydrogen or halogeno, or alternatively X1 and X2 may be united to form lower alkylenedioxy; Q is pyridyl or quinolyl; R1 is hydrogen or optionally substituted lower alkyl or aryl; R2 is hydrogen, lower alkyl, or aralkyl; R3 is hydrogen, an organic sulfonyl group, or -C(:Y)-R4; R4 is hydrogen or an organic residue; and Y is oxygen or sulfur, with the proviso that when R3 is hydrogen, R1 is not hydrogen and R2 is hydrogen] are prepared These compds. exhibit excellent p38MAP kinase inhibiting activities and are useful in the prevention or treatment of diseases related to tumor necrosis factor α, interleukin 1, interleukin 6 or cyclooxygenase II. These diseases include chronic articular rheumatism, multiple sclerosis, osteoarthritis, psoriasis, HIV, asthma, septic shock, inflammatory enteric disease, Crohn's disease, Alzheimer's disease, diabetes, cachexia, osteoporosis, graft-vs.-host disease, adult respiratory distress syndrome, arteriosclerosis, gout, glomerulus nephritis (glomerulonephritis), ischemic heart failure, ulcerative colitis, septicemia, cerebral malaria, restenosis, hepatitis, systemic lupus erythematosus, thrombosis, bone resorption disease, chronic pulmonary inflammation disease, heart or kidney reperfusion disorder, cancers, Reiter's syndrome, imminent abortion, eczema, homograft rejection, seizure, fever, Behcet's disease, neuralgia, meningitis, sunburn, contact dermatitis, acute synovitis, myelitis, muscle degeneration, neovascularization, conjunctivitis, psoriatic arthritis, viral myocarditis, pancreatitis, blastoma, bleeding, arthritis, endotoxin shock, parasitic infection, tuberculosis, myocardial infarction, Hansen's disease, diabetic conjunctivitis, irritable bowel syndrome, transplant rejection, burn, bronchitis, ischemic heart disease, eclampsia, pneumonia, remission of swelling, low back pain (lumbago), myelitis, pharyngolaryngitis, Kawasaki disease, or atopic dermatitis. Thus, 306 mg Et3N was added to a suspension of 254 mg 3-amino-5-(4-fluorophenyl)-4-(4- pyridyl)pyrazone in 20 mL THF, followed by adding dropwise a solution of 464 mg phenylacetyl chloride in 5 mL THF, and the resulting mixture was stirred at room temperature for 3 h to give 22% 5-(4-fluorophenyl)-3-phenylacetylamino-4- (4-pyridyl)pyrazole (II). II and 5-(2-chlorophenylacetylamino)-3-(4- fluorophenyl)-1-methyl-4-(4-pyridyl)pyrazole showed IC50 of 0.042 and 0.0000088 μg/mL against p38MAP kinase.

IT 277747-50-9P 277747-51-0P 277747-73-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aminopyrazole derivs. as p38MAP kinase inhibitors for treatment of prevention of diseases related to tumor necrosis factor α, interleukin 1, interleukin 6 or cyclooxygenase II)

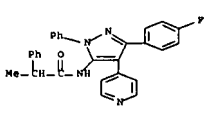
RN 277747-50-9 HCAPLUS
CN Benzeneacetamide, 2-chloro-N-[3-(4-fluorophenyl)-1-phenyl-4-(4-pyridinyl)-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A



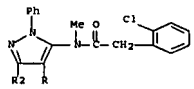
PAGE 2-A

RN 277747-51-0 HCAPLUS
CN Benzeneacetamide, N-[3-(4-fluorophenyl)-1-phenyl-4-(4-pyridinyl)-1H-pyrazol-5-yl]-α-methyl- (9CI) (CA INDEX NAME)



RN 277747-73-6 HCAPLUS
CN Benzeneacetamide, 2-chloro-N-[3-(4-fluorophenyl)-1-phenyl-4-(4-pyridinyl)-1H-pyrazol-5-yl]-N-methyl- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 25 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:699078 HCAPLUS Full-text
DOCUMENT NUMBER: 131:317778
TITLE: Phosphate derivatives for treatment of nephritis
INVENTOR(S): Miyata, Kazuyoshi; Tsuda, Yoshihiko; Koji, Yasuo; Kuroki, Morihisa; Sakai, Yasuhiro; Mukai, Kiyoshi; Hashimoto, Kinji; Kori, Hideaki
PATENT ASSIGNEE(S): Ohtsuka Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 19 pp.
CODEN: JKXXAP
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

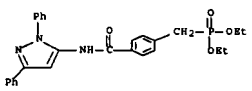
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11302177	A	19991102	JP 1998-116645	19980427 <--
PRIORITY APPLN. INFO.:			JP 1998-116645	19980427
OTHER SOURCE(S):	MARPAT 131:317778			

AB Phosphate derivs. (Markush's structures given) are claimed for treatment of nephritis. The derivs. inhibited mesangium cell proliferation in vitro. Examples of tablets, capsules, and granules were formulated.

IT 169293-99-6
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(phosphate derivs. for treatment of nephritis)

RN 169293-99-6 HCAPLUS
CN Phosphonic acid, [[4-[[(1,3-diphenyl-1H-pyrazol-5-

yl)amino]carbonyl]phenyl]methyl]-, diethyl ester (9CI) (CA INDEX NAME)

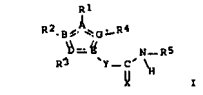


L5 ANSWER 26 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:311199 HCAPLUS Full-text
DOCUMENT NUMBER: 130:325145
TITLE: Preparation of aromatic heterocyclic compounds as antiinflammatory agents
INVENTOR(S): Regan, John R.; Cirillo, Pier F.; Hickey, Eugene R.; Moss, Neil; Cywin, Charles L.; Pargellis, Christopher; Gilmore, Thomas A.
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 87 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9923091	A1	19990514	WO 1998-US22907	19981029 <--
W: AU, BG, BR, BY, CA, CN, CZ, HR, HU, ID, IL, JP, KR, KZ, LT, LV, MX, NO, NZ, PL, RO, RU, TR, UA, UZ, VN, YU				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2308428	A1	19990514	CA 1998-2308428	19981029 <--
AU 9913675	A	19990524	AU 1999-13675	19981029 <--
US 6080763	A	20000627	US 1998-181743	19981029 <--
EP 1028953	A1	20000823	EP 1998-957405	19981029 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2001521934	T	20011113	JP 2000-518962	19981029 <--
EP 1473292	A1	20041103	EP 2004-8840	19981029
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				
US 6228881	B1	20010508	US 1999-461446	19991214 <--
US 2001039290	A1	20011108	US 2001-808084	20010314 <--

PRIORITY APPLN. INFO.:
US 1997-64102P P 19971103
EP 1998-957405 A3 19981029
US 1998-181743 A3 19981029
WO 1998-US22907 W 19981029
US 1999-461446 A3 19991214

OTHER SOURCE(S): MARPAT 130:325145
GI



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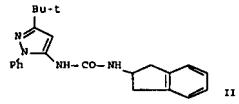
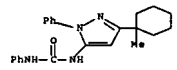


II

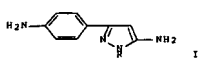
AB The title compds. I [A = C, N; B = C, N, O, etc.; D = C, N, S; E = C, N; G = C, S, N; X = S, O, etc.; Y = NH, etc.; R1 = (un)substituted, (partially or fully halogenated) alkyl, etc.; R2 is H, (partially or fully halogenated) alkyl, etc., when B is C or N; R3 is Ph, naphthyl, etc., when D is C or N; or R1R2 = fused Ph or pyridinyl ring; or R2R3 = fused Ph or pyridinyl ring; R4 is H, (partially or fully halogenated) alkyl when G is C or N; R5 is Ph, naphthyl, heteroaryl, etc.] are prepared I inhibit production of cytokines involved in immunoregulation and inflammation such as interleukin-1 and tumor necrosis factor. Pyrazole derivative II was prepared from phenylhydrazine and 4,4-dimethyl-3-oxopentanenitrile. Compds. of this invention had IC50 < 10 μM against TNF production in an in vitro assay using THP cells.
IT 223724-97-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aromatic heterocyclic compds. as antiinflammatory agents)
RN 223724-97-8 HCAPLUS
CN Urea, N-[3-(1-methylcyclohexyl)-1-phenyl-1H-pyrazol-5-yl]-N'-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

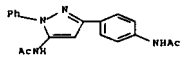
L5 ANSWER 27 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:126025 HCAPLUS Full-text
DOCUMENT NUMBER: 130:311726
TITLE: Acyl derivatives of 3-(p-aminophenyl)-5-aminopyrazole and its N(1)-substituted derivatives
AUTHOR(S): Nam, N. L.; Grandberg, I. I.; Sorokin, V. I.
CORPORATE SOURCE: Timiryazevsk. Sel'skokhoz. Akad., Russia
SOURCE: Izvestiya Timiryazevskoi Sel'skokhozyaistvennoi Akademii (1999), (3), 201-211
CODEN: ITSAA7; ISSN: 0021-342X
PUBLISHER: Izdatel'stvo MSKhA
DOCUMENT TYPE: Journal

LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 130:311726
GI

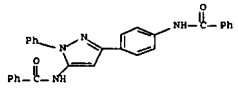


I

AB Title compds. such as I (R = H, Me, Ph, o-tolyl, p-tolyl) were acylated on both primary amino groups.
IT 94254-75-8P 223518-55-6P 223518-59-0P
223518-63-6P 223518-65-8P 223518-69-2P
223518-74-9P 223518-76-1P 223518-80-7P
223518-85-2P 223518-87-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 94254-75-8 HCAPLUS
CN Acetamide, N-[3-[4-(acetylamino)phenyl]-1-phenyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

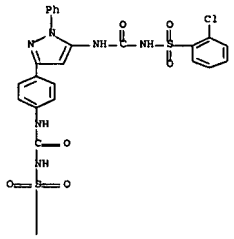


RN 223518-55-6 HCAPLUS
CN Benzamide, N-[3-[4-(benzoylamino)phenyl]-1-phenyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)



RN 223518-59-0 HCAPLUS
CN Benzenesulfonamide, 2-chloro-N-[[[3-[4-[[[[(2-chlorophenyl]sulfonyl]amino]carbonyl]amino]phenyl]-1-phenyl-1H-pyrazol-5-yl]amino]carbonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



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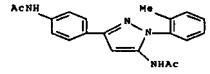
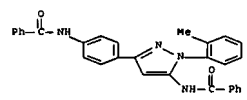
RN 223518-63-6 HCAPLUS
CN Acetamide, N-[4-[5-(acetylamino)-1-(2-methylphenyl)-1H-pyrazol-3-yl]phenyl]- (9CI) (CA INDEX NAME)

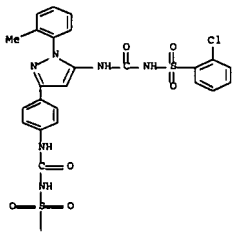


RN 223518-65-8 HCAPLUS
CN Benzamide, N-[4-[5-(benzoylamino)-1-(2-methylphenyl)-1H-pyrazol-3-yl]phenyl]- (9CI) (CA INDEX NAME)



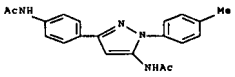
RN 223518-69-2 HCAPLUS
CN Benzenesulfonamide, 2-chloro-N-[[[4-[5-[[[[(2-chlorophenyl)sulfonyl]amino]carbonyl]amino]-1-(2-methylphenyl)-1H-pyrazol-3-yl]phenyl]amino]carbonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

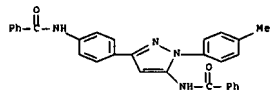


PAGE 2-A

RN 223518-74-9 HCAPLUS
CN Acetamide, N-[4-[5-(acetylamino)-1-(4-methylphenyl)-1H-pyrazol-3-yl]phenyl]- (9CI) (CA INDEX NAME)

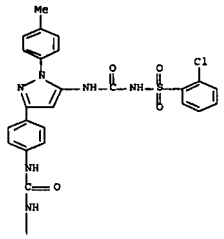


RN 223518-76-1 HCAPLUS
CN Benzamide, N-[4-[5-(benzoylamino)-1-(4-methylphenyl)-1H-pyrazol-3-yl]phenyl]- (9CI) (CA INDEX NAME)



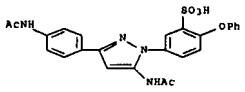
RN 223518-80-7 HCAPLUS
CN Benzenesulfonamide, 2-chloro-N-[[[4-[5-[[[[(2-chlorophenyl)sulfonyl]amino]carbonyl]amino]-1-(4-methylphenyl)-1H-pyrazol-3-yl]phenyl]amino]carbonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

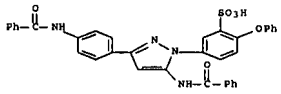


PAGE 2-A

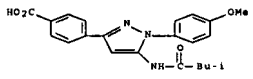
RN 223518-85-2 HCAPLUS
CN Benzenesulfonic acid, 5-[5-(acetylamino)-3-[4-(acetylamino)phenyl]-1H-pyrazol-1-yl]-2-phenoxy- (9CI) (CA INDEX NAME)



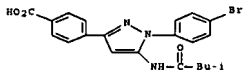
RN 223518-87-4 HCAPLUS
CN Benzenesulfonic acid, 5-[5-(benzoylamino)-3-[4-(benzoylamino)phenyl]-1H-pyrazol-1-yl]-2-phenoxy- (9CI) (CA INDEX NAME)



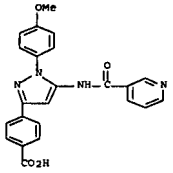
L5 ANSWER 28 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:24217 HCAPLUS Full-text
DOCUMENT NUMBER: 128:88829
TITLE: Solid phase synthesis of 5-aminopyrazoles and derivatives
AUTHOR(S): Watson, Stephen P.; Wilson, Richard D.; Judd, Duncan B.; Richards, Stephen A.
CORPORATE SOURCE: Discovery Chemistry, Units, GlaxoWellcome Medicines Research Centre, Stevenage, SG1 2NY, UK
SOURCE: Tetrahedron Letters (1997), 38(52), 9065-9068
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The development of a novel solid phase synthesis of some 5-aminopyrazoles and derivs. is described. Reaction of hydrazines with solid supported β-keto nitrile, 4-HO2CC6H4COCH2CN, affords 5-aminopyrazoles the amino group of which is readily acylated or sulfonylated. Generation of the solid supported β-keto nitrile is non-trivial and represents a key step in the overall synthesis.
IT 201139-22-2P 201139-23-3P 201139-26-6P
201139-27-7P 201139-30-2P 201139-31-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(solid phase synthesis of 5-aminopyrazoles)
RN 201139-22-2 HCAPLUS
CN Benzoic acid, 4-[1-(4-methoxyphenyl)-5-[(3-methyl-1-oxobutyl)amino]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



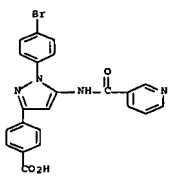
RN 201139-23-3 HCAPLUS
CN Benzoic acid, 4-[1-(4-bromophenyl)-5-[(3-methyl-1-oxobutyl)amino]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



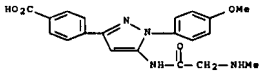
RN 201139-26-6 HCAPLUS
CN Benzoic acid, 4-[1-(4-methoxyphenyl)-5-[(3-pyridinylcarbonyl)amino]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



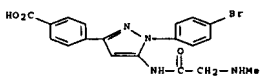
RN 201139-27-7 HCAPLUS
CN Benzoic acid, 4-[1-(4-bromophenyl)-5-[(3-pyridinylcarbonyl)amino]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



RN 201139-30-2 HCAPLUS
CN Benzoic acid, 4-[1-(4-methoxyphenyl)-5-[[(methylamino)acetyl]amino]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



RN 201139-31-3 HCAPLUS
CN Benzoic acid, 4-[1-(4-bromophenyl)-5-[[(methylamino)acetyl]amino]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



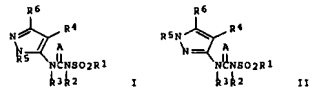
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 29 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:579703 HCAPLUS Full-text
DOCUMENT NUMBER: 127:205576
TITLE: Preparation of sulfonylureidopyrazole derivatives as endothelin converter enzyme inhibitors
INVENTOR(S): Matsushita, Kayo; Hasegawa, Hirohiko; Kuribayashi, Yoshikazu; Ohashi, Naohito
PATENT ASSIGNEE(S): Sumitomo Pharmaceuticals Co., Ltd., Japan; Matsushita, Kayo; Hasegawa, Hirohiko; Kuribayashi, Yoshikazu; Ohashi, Naohito
SOURCE: PCT Int. Appl., 260 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

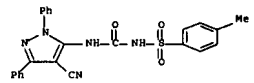
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9730978	A1	19970828	WO 1997-JP532	19970225 <--
W: AU, CA, CN, KR, NZ, RU, US				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
JP 10007658	A	19980113	JP 1997-56883	19970224 <--
CA 2247286	A1	19970828	CA 1997-2247286	19970225 <--
AU 9717354	A	19970910	AU 1997-17354	19970225 <--
EP 885890	A1	19981223	EP 1997-904634	19970225 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, SE, PT, IE, FI				

PRIORITY APPLN. INFO.: JP 1996-65498 A 19960226
WO 1997-JP532 W 19970225

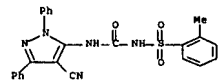
OTHER SOURCE(S): MARPAT 127:205576
GI



AB The title compds. (I and II; A = O, S; R1 = alkyl, alkenyl, alkynyl, cycloalkyl, etc.; R2, R3 = H, aryl, alkyl, alkenyl, alkynyl, cycloalkyl, etc.; R4, R6 = H, halo, NH2, NO2, alkyl, alkenyl, alkynyl, cycloalkyl, etc; R5 = heterocyclyl, H, aryl, alkyl, alkenyl, alkynyl, cycloalkyl, etc.) are prepared I and II, having inhibitory effects on endothelin converter enzyme (ECE), are useful in the prevention and treatment of various circulatory disease, bronchial contraction, nervous disorder, hyposecretion, vascular lesions, various ulcers, etc. Thus, 5-amino-4-cyano-1-phenyl-(1H)-pyrazole was reacted with 4-toluenesulfonyl isocyanate to give 84.1% I (R1 = 4-MeC6H4, R2 = R3 = R6 = H, R4 = CN, R5 = Ph), which showed IC50 of 4.6 μM against ECE.
IT 194542-43-3P 194542-44-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of sulfonylureidopyrazole derivs. as endothelin converter enzyme inhibitors)
RN 194542-43-3 HCAPLUS
CN Benzenesulfonamide, N-[[(4-cyano-1,3-diphenyl-1H-pyrazol-5-yl)amino]carbonyl]-4-methyl- (9CI) (CA INDEX NAME)

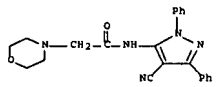


RN 194542-44-4 HCAPLUS
CN Benzenesulfonamide, N-[[(4-cyano-1,3-diphenyl-1H-pyrazol-5-yl)amino]carbonyl]-2-methyl- (9CI) (CA INDEX NAME)

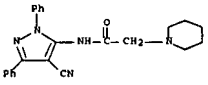


L5 ANSWER 30 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:239113 HCAPLUS Full-text
DOCUMENT NUMBER: 126:343473
TITLE: 3-Amino-2(1H)-quinolones by cyclization of N-acylated anthranilic acid derivatives

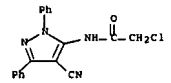
AUTHOR(S): Rehwald, Matthias; Gewald, Karl; Lankau, Hans-Joachim; Unverferth, Klaus
CORPORATE SOURCE: Inst. Org. Chem., Tech. Univ. Dresden, Dresden, D-01062, Germany
SOURCE: Heterocycles (1997), 45(3), 483-492
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 126:343473
AB Reaction of secondary amines with N-(iodoacetyl)anthranilic acid derivs., 2-(iodoacetylamino)acetophenone and 2-(iodoacetylamino)benzophenone yielded 3-amino-2(1H)-quinolones in two steps. Analogously heterocondensed 5-amino-6(7H)-pyrazolo[5,4-b]pyridones were prepared Hydroxyquinolines were subjected to Cl/OH exchange to give chloroquinolines, which are convenient for consecutive reactions.
IT 189757-41-3P 189757-42-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of)
RN 189757-41-3 HCAPLUS
CN 4-Morpholineacetamide, N-(4-cyano-1,3-diphenyl-1H-pyrazol-5-yl)- (9CI) (CA INDEX NAME)



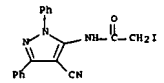
RN 189757-42-4 HCAPLUS
CN 1-Piperidineacetamide, N-(4-cyano-1,3-diphenyl-1H-pyrazol-5-yl)- (9CI) (CA INDEX NAME)



IT 189757-39-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of aminoquinolones by cyclization of N-acylated anthranilic acid derivs.)
RN 189757-39-9 HCAPLUS
CN Acetamide, 2-chloro-N-(4-cyano-1,3-diphenyl-1H-pyrazol-5-yl)- (9CI) (CA INDEX NAME)



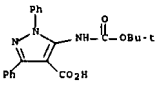
IT 189757-40-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of aminoquinolones by cyclization of N-acylated anthranilic acid derivs.)
RN 189757-40-2 HCAPLUS
CN Acetamide, N-(4-cyano-1,3-diphenyl-1H-pyrazol-5-yl)-2-iodo- (9CI) (CA INDEX NAME)



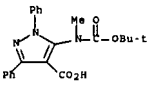
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=>
=> d ibib abs hitstr 31-50

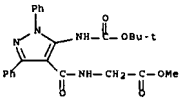
L5 ANSWER 31 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:860793 HCAPLUS Full-text
DOCUMENT NUMBER: 124:87730
TITLE: Synthesis of cyclodipeptides from β-pyrazolic amino acids
AUTHOR(S): El Mahdi, Ouafaa; Lavergne, Jean-Pierre; Viallefont, Philippe; Akssira, Mohamed; Sedqui, Ahmed
CORPORATE SOURCE: Lab. Amino-Acides Peptides, Univ. Montpellier II, Montpellier, 34095, Fr.
SOURCE: Bulletin de la Societe Chimique de France (1995), 132(7), 675-80
CODEN: BSCFAS; ISSN: 0037-8968
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: French
OTHER SOURCE(S): CASREACT 124:87730
AB Seven-membered ring cyclopeptides [pyrazolo[3,4-e][1,4]diazepine-4,7- diones] were prepared by a two-step procedure from β-pyrazolic amino acids.
IT 165676-72-2 172506-48-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of cyclodipeptides from pyrazolic amino acids)
RN 165676-72-2 HCAPLUS
CN 1H-Pyrazole-4-carboxylic acid, 5-[[(1,1-dimethylethoxy)carbonyl]amino]-1,3-diphenyl- (9CI) (CA INDEX NAME)



RN 172506-48-8 HCAPLUS
CN 1H-Pyrazole-4-carboxylic acid, 5-[[(1,1-dimethylethoxy)carbonyl]methylamino]-1,3-diphenyl- (9CI) (CA INDEX NAME)

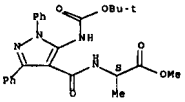


IT 172506-53-5P 172506-54-6P 172506-55-7P
172506-56-8P 172506-57-9P 172506-58-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of cyclodipeptides from pyrazolic amino acids)
RN 172506-53-5 HCAPLUS
CN Glycine, N-[[5-[[(1,1-dimethylethoxy)carbonyl]amino]-1,3-diphenyl-1H-pyrazol-4-yl]carbonyl]-, methyl ester (9CI) (CA INDEX NAME)



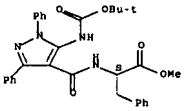
RN 172506-54-6 HCAPLUS
CN L-Alanine, N-[[5-[[(1,1-dimethylethoxy)carbonyl]amino]-1,3-diphenyl-1H-pyrazol-4-yl]carbonyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

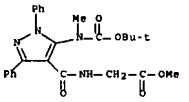


RN 172506-55-7 HCAPLUS
CN L-Phenylalanine, N-[[5-[[(1,1-dimethylethoxy)carbonyl]amino]-1,3-diphenyl-1H-pyrazol-4-yl]carbonyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

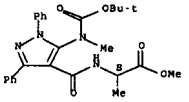


RN 172506-56-8 HCAPLUS
CN Glycine, N-[[5-[[(1,1-dimethylethoxy)carbonyl]methylamino]-1,3-diphenyl-1H-pyrazol-4-yl]carbonyl]-, methyl ester (9CI) (CA INDEX NAME)



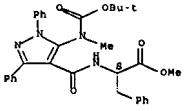
RN 172506-57-9 HCAPLUS
CN L-Alanine, N-[[5-[[(1,1-dimethylethoxy)carbonyl]methylamino]-1,3-diphenyl-1H-pyrazol-4-yl]carbonyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

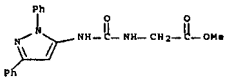


RN 172506-58-0 HCAPLUS
CN L-Phenylalanine, N-[[5-[[(1,1-dimethylethoxy)carbonyl]methylamino]-1,3-diphenyl-1H-pyrazol-4-yl]carbonyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 172506-60-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of cyclodipeptides from pyrazolic amino acids)
RN 172506-60-4 HCAPLUS
CN Glycine, N-[[(1,3-diphenyl-1H-pyrazol-5-yl)amino]carbonyl]-, methyl ester (9CI) (CA INDEX NAME)



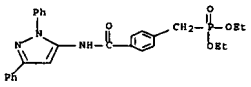
L5 ANSWER 32 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:856442 HCAPLUS Full-text
DOCUMENT NUMBER: 123:286296
TITLE: Preparation of phosphonic diester derivatives as antihyperlipidemics and antidiabetics
INVENTOR(S): Shoji, Yasuo; Myata, Kazuyoshi; Kuroki, Yasuhisa; Tsuda, Yoshihiko; Tsutsumi, Kazuhiko; Inoe, Yasuhide
PATENT ASSIGNEE(S): Otsuka Pharma Co Ltd, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07188269	A	19950725	JP 1993-330166	19931227 <--
JP 3156026	B2	20010416		

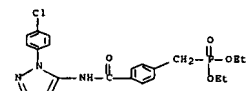
PRIORITY APPLN. INFO.: JP 1993-330166 19931227
OTHER SOURCE(S): MARPAT 123:286296

AB BNHAC6H4CH2P(O)R1R2 [R1, R2 = lower alkoxy, Ph; A = CO, CS, SO2; B is selected from heterocyclyl of (a) (halo-substituted) pyridine containing 1-2 of (halo-substituted) lower alkyl, CONH2, NO2, cyano, or lower alkanyloxyl; (b) pyridine 1-oxide (containing 1-2 of (halo-substituted) lower alkyl, halo, or cyano); (c) pyrimidine containing 1-2 of lower alkyl, halo, or lower alkylthio; (d) pyrazine (containing 1-2 halo); (e) isoxazole containing 1-2 of (halo)phenyl, lower alkoxyphenyl, lower alkylphenyl, thienyl, phenylsulfonyl, or OH, or halo and lower alkyl; (f) pyrazole or 3-pyrazolone (containing 1-3 of lower (phenyl)alkyl, (halo)phenyl, cyano, CONH2, or thiocyanate); (g) (lower alkyl- or halo-substituted) quinoline 1-oxide; (h) 1 or 2 lower alkyl-substituted 1,8-naphthyridine] are prepared as antihyperlipidemics and antidiabetics (no data). Thus, a mixture of 3.1 g 2-amino-5-cyanopyridine-HCl and pyridine in CH2Cl2 was treated dropwise

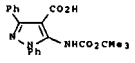
with a solution of 6.4 g 4-[(diethoxyphosphoryl)methyl]benzoyl chloride in CH2Cl2 under ice cooling, then treated at room temperature for 10 h to give 5.1 g diisopropyl 4-[N-(5-cyano-2-pyridyl)carbamoyl]benzylphosphonate.
IT 169293-99-6P 169294-03-5P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heterocyclyl-containing phosphonate diesters as antihyperlipidemics and antidiabetics)
RN 169293-99-6 HCAPLUS
CN Phosphonic acid, [[4-[[(1,3-diphenyl-1H-pyrazol-5-yl)amino]carbonyl]phenyl]methyl]-, diethyl ester (9CI) (CA INDEX NAME)



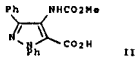
RN 169294-03-5 HCAPLUS
CN Phosphonic acid, [[4-[[[1-(4-chlorophenyl)-3-phenyl-1H-pyrazol-5-yl]amino]carbonyl]phenyl]methyl]-, diethyl ester (9CI) (CA INDEX NAME)



L5 ANSWER 33 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:376058 HCAPLUS Full-text
DOCUMENT NUMBER: 123:111925
TITLE: Synthesis of pyrazolic amino acids
AUTHOR(S): El Mahdi, O.; Lavergne, J.-P.; Viallefont, Ph.; Aknsira, M.
CORPORATE SOURCE: Lab. Amino Acides Peptides, Univ. Montpellier II, Montpellier, 34095, Fr.
SOURCE: Bulletin des Societes Chimiques Belges (1995), 104(1), 31-7
CODEN: BSCBAG; ISSN: 0037-9646
PUBLISHER: Societe Chimique Belges
DOCUMENT TYPE: Journal
LANGUAGE: French
GI



I



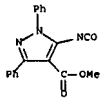
II

AB Two regioisomeric pyrazolic amino acids I and II were prepd from di-Me 1,3-diphenyl-1H-pyrazole-4,5-dicarboxylate.

IT 165676-68-6P 165676-70-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of regioisomeric pyrazole amino acids)

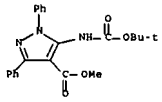
RN 165676-68-6 HCAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 5-isocyanato-1,3-diphenyl-, methyl ester (9CI) (CA INDEX NAME)



RN 165676-70-0 HCAPLUS

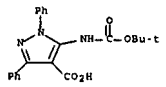
CN 1H-Pyrazole-4-carboxylic acid, 5-[[(1,1-dimethylethoxy)carbonyl]amino]-1,3-diphenyl-, methyl ester (9CI) (CA INDEX NAME)



IT 165676-72-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of regioisomeric pyrazole amino acids)

RN 165676-72-2 HCAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 5-[[(1,1-dimethylethoxy)carbonyl]amino]-1,3-diphenyl- (9CI) (CA INDEX NAME)



L5 ANSWER 34 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1994:270224 HCAPLUS Full-text

DOCUMENT NUMBER: 120:270224

TITLE: Synthesis and rearrangement of pyrazolylamino alcohols

AUTHOR(S): Abdallah, Magda A.; Abbas, Ikhlass M.; Mosselhi, Mosselhi A. N.; Albar, Hassan A.; Shawali, Ahmad S.

CORPORATE SOURCE: Fac. Sci., Univ. Cairo, Giza, Egypt

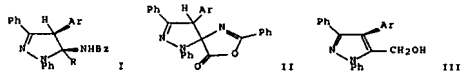
SOURCE: Journal of Chemical Research, Synopses (1994), (2), 76-7
CODEN: JRPSDC; ISSN: 0308-2342

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 120:270224

GI



I II III

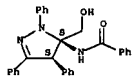
AB 4-Aryl-5-benzoylamino-5-hydroxymethyl-1,3-diphenyl-2-pyrazolines I (R = CH2OH, Ar = Ph, 4-MeC6H4, 4-MeOC6H4, 4-ClC6H4) were prepared by LiAlH4 reduction of either the spiropyrazolines II or the corresponding pyrazoline esters I (R = CO2Me); treatment of I (R = CH2OH) with hydrochloric acid in dioxane at room temperature, gave 4-aryl-5-hydroxymethyl-1,3-diphenylpyrazoles III.

IT 154594-04-4P 154594-05-5P 154594-06-6P
154594-07-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and rearrangement of)

RN 154594-04-4 HCAPLUS

CN Benzamide, N-[4,5-dihydro-5-(hydroxymethyl)-1,3,4-triphenyl-1H-pyrazol-5-yl]-, cis- (9CI) (CA INDEX NAME)

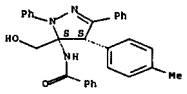
Relative stereochemistry.



RN 154594-05-5 HCAPLUS

CN Benzamide, N-[4,5-dihydro-5-(hydroxymethyl)-4-(4-methylphenyl)-1,3-diphenyl-1H-pyrazol-5-yl]-, cis- (9CI) (CA INDEX NAME)

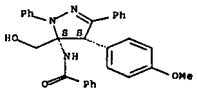
Relative stereochemistry.



RN 154594-06-6 HCAPLUS

CN Benzamide, N-[4,5-dihydro-5-(hydroxymethyl)-4-(4-methoxyphenyl)-1,3-diphenyl-1H-pyrazol-5-yl]-, cis- (9CI) (CA INDEX NAME)

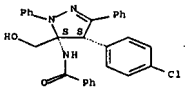
Relative stereochemistry.



RN 154594-07-7 HCAPLUS

CN Benzamide, N-[4-(4-chlorophenyl)-4,5-dihydro-5-(hydroxymethyl)-1,3-diphenyl-1H-pyrazol-5-yl]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

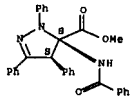


IT 129624-41-5 145383-21-7 145383-22-8
154594-03-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of)

RN 129624-41-5 HCAPLUS

CN 1H-Pyrazole-5-carboxylic acid, 5-(benzoylamino)-4,5-dihydro-1,3,4-triphenyl-, methyl ester, cis- (9CI) (CA INDEX NAME)

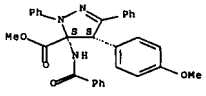
Relative stereochemistry.



RN 145383-21-7 HCAPLUS

CN 1H-Pyrazole-5-carboxylic acid, 5-(benzoylamino)-4,5-dihydro-4-(4-methoxyphenyl)-1,3-diphenyl-, methyl ester, cis- (9CI) (CA INDEX NAME)

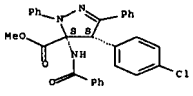
Relative stereochemistry.



RN 145383-22-8 HCAPLUS

CN 1H-Pyrazole-5-carboxylic acid, 5-(benzoylamino)-4-(4-chlorophenyl)-4,5-dihydro-1,3-diphenyl-, methyl ester, cis- (9CI) (CA INDEX NAME)

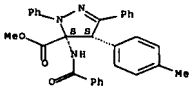
Relative stereochemistry.



RN 154594-03-3 HCAPLUS

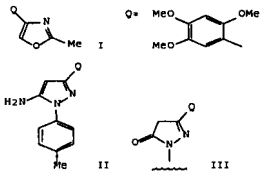
CN 1H-Pyrazole-5-carboxylic acid, 5-(benzoylamino)-4,5-dihydro-4-(4-methylphenyl)-1,3-diphenyl-, methyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

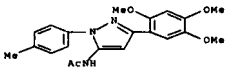


L5 ANSWER 35 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1994:217403 HCAPLUS Full-text
DOCUMENT NUMBER: 120:217403
TITLE: Synthesis and spectroscopy of new substituted arylazoles
AUTHOR(S): Sanchez-Viesca, F.; Gomez, Maria R.
CORPORATE SOURCE: Fac. Quim., UNAM, Mexico City, 04510, Mex.
SOURCE: Revista Latinoamericana de Quimica (1991), 22(3), 85-9
CODEN: RLAQA8; ISSN: 0370-5943
DOCUMENT TYPE: Journal
LANGUAGE: Spanish
OTHER SOURCE(S): CASREACT 120:217403
GI

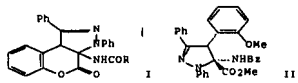


AB Methyl(trimethoxyphenyl)oxazole I could not be prepared by cyclocondensation of an α-halo ketone and an amide, but was prepared in 72% yield from acyloin ester QCOCH2OAc and NH4OAc in AcOH. I could not be converted to its imidazole analog, which also could not be prepared by other routes. This is presumably due to special reactivity of such 2,4,5-trimethoxyphenyl compds., as seen previously. On the other hand, cyclization of QCOCH2CN with p-MeC6H4NHNH2.HCl gave 70% aminopyrazole derivative II, which was N-acetylated in 74% yield. Similar cyclization of QCOCH2CONH2 gave 97% pyrazolinone III. Some characteristic IR, 1H-NMR, and mass spectral data are given and discussed.
IT 153981-93-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of aryloxazole and arylpyrazoles)
RN 153981-93-2 HCAPLUS
CN Acetamide, N-[1-(4-methylphenyl)-3-(2,4,5-trimethoxyphenyl)-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)



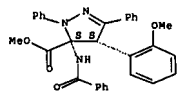
L5 ANSWER 36 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:30710 HCAPLUS Full-text
DOCUMENT NUMBER: 120:30710
TITLE: Synthesis of aminopyrazolecarboxylic acid derivatives

AUTHOR(S): Shawali, Ahmad S.; Hassaneen, Hamdi M.; Albart, Hassan A.; Abdelhamid, Hyam A.
CORPORATE SOURCE: Fac. Sci., Univ. Cairo, Giza, Egypt
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1993), 32B(7), 795-6
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 120:30710
GI

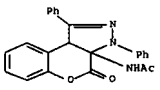


AB Diphenylnitrilimine adds regioselectively to 3-acylaminocoumarins and Me α-acylamino-o-methoxycinnamate to yield exclusively the cycloadducts I (R = Me, Ph) and II, resp. I were converted into II by their treatment with KOH and di-Me sulfate in methanol. The regiochem. of the cycloadducts have been confirmed by their conversion to the known 1,3-diphenylchromeno[3,4-c]pyrazol-4-(3H)-one and Me 1,3-diphenyl-4-(o- methoxyphenyl)-pyrazole-5-carboxylate, resp.
IT 145383-20-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and elimination reaction of)
RN 145383-20-6 HCAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 5-(benzoylamino)-4,5-dihydro-4-(2-methoxyphenyl)-1,3-diphenyl-, methyl ester, cis- (9CI) (CA INDEX NAME)

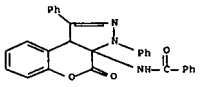
Relative stereochemistry.



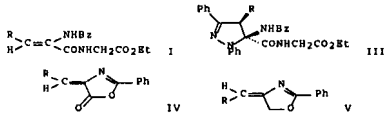
IT 151806-42-7P 151806-43-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and ring cleavage of)
RN 151806-42-7 HCAPLUS
CN Acetamide, N-(3,9b-dihydro-4-oxo-1,3-diphenyl[1]benzopyrano[3,4-c]pyrazol-3a(4H)-yl)- (9CI) (CA INDEX NAME)



RN 151806-43-8 HCAPLUS
CN Benzamide, N-(3,9b-dihydro-4-oxo-1,3-diphenyl[1]benzopyrano[3,4-c]pyrazol-3a(4H)-yl)- (9CI) (CA INDEX NAME)



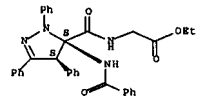
L5 ANSWER 37 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1993:581191 HCAPLUS Full-text
DOCUMENT NUMBER: 119:181191
TITLE: 1,3-Dipolar cycloaddition of benzonitrilium N-phenylimide to didehydropeptides
AUTHOR(S): Abdallah, Magda A.; Albar, Hassan A.; Shawali, Ahmad S.
CORPORATE SOURCE: Fac. Sci., Univ. Cairo, Giza, Egypt
SOURCE: Journal of Chemical Research, Synopses (1993), (5), 182-3
CODEN: JRPSDC; ISSN: 0308-2342
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 119:181191
GI



AB Didehydropeptides I (Ar = Ph, 4-MeOC6H4, 4-MeC6H4, 4-ClC6H4, 4-O2NC6H4, 3,4-methylenedioxyphenyl) underwent a regioselective 1,3-dipolar cycloaddn. reaction with benzonitrilium N-phenylimide PhC.tplbond.N+N-Ph (II) to give cycloadducts III. I were obtained by the ring cleavage of (Z)-oxazolones IV or (E)-oxazolones V with H-Gly-OEt.HCl in the presence of Et3N in DMF. II was generated in situ from PhC(:NNHPh)Cl by treatment with Et3N.

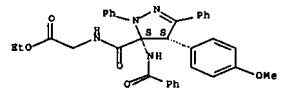
IT 150330-79-3P 150330-80-6P 150330-81-7P
150330-82-8P 150330-83-9P 150330-84-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by regioselective 1,3-dipolar cycloaddn. reaction of benzonitrilium phenylimide with didehydropeptide)
RN 150330-79-3 HCAPLUS
CN Glycine, N-[(5-(benzoylamino)-4,5-dihydro-1,3,4-triphenyl-1H-pyrazol-5-yl]carbonyl]-, ethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



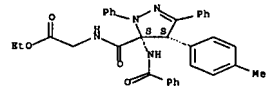
RN 150330-80-6 HCAPLUS
CN Glycine, N-[(5-(benzoylamino)-4,5-dihydro-4-(4-methoxyphenyl)-1,3-diphenyl-1H-pyrazol-5-yl]carbonyl]-, ethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



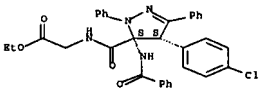
RN 150330-81-7 HCAPLUS
CN Glycine, N-[(5-(benzoylamino)-4,5-dihydro-4-(4-methylphenyl)-1,3-diphenyl-1H-pyrazol-5-yl]carbonyl]-, ethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



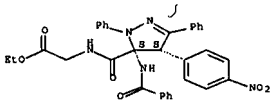
RN 150330-82-8 HCAPLUS
CN Glycine, N-[(5-(benzoylamino)-4-(4-chlorophenyl)-4,5-dihydro-1,3-diphenyl-1H-pyrazol-5-yl]carbonyl]-, ethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



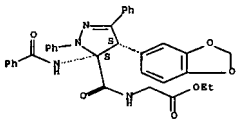
RN 150330-83-9 HCAPLUS
CN Glycine, N-[[5-(benzoylamino)-4,5-dihydro-4-(4-nitrophenyl)-1,3-diphenyl-1H-pyrazol-5-yl]carbonyl]-, ethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

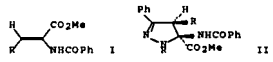


RN 150330-84-0 HCAPLUS
CN Glycine, N-[[4-(1,3-benzodioxol-5-yl)-5-(benzoylamino)-4,5-dihydro-1,3-diphenyl-1H-pyrazol-5-yl]carbonyl]-, ethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

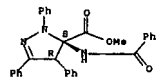


L5 ANSWER 38 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1993:59626 HCAPLUS Full-text
DOCUMENT NUMBER: 118:59626
TITLE: 1,3-Dipolar cycloaddition reactions of diphenylnitrilimine with esters of α,β-didehydro amino acids
AUTHOR(S): Shawali, Ahmad S.; Fahmi, Abdelgawad A.; Hassaneen, Hamdi M.; Abdallah, Magda A.; Abdelhamid, Hyam A.
CORPORATE SOURCE: Fac. Sci., Univ. Cairo, Giza, Egypt
SOURCE: Journal of Chemical Research, Synopses (1992), (11), 360-1
CODEN: JRPSDC; ISSN: 0308-2342
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 118:59626
GI



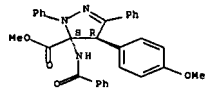
AB Diphenylnitrilimine adds regioselectively to the carbon-carbon double bond of Me β-aryl-N-benzoyl-α,β-didehydroalaninates I (R = aryl) to afford the pyrazoline deriva. II (R = aryl). The regiochem. of the latter cycloadducts was evidenced chemical by their conversion to the known 1,3,4-triarylpyrazole-5-carboxylates and by their alternative synthesis from the recently reported spiropyrazoles. The 1H NMR spectral data of II were compatible with their assigned structure.
IT 139285-17-9P 145383-27-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and attempted thermolysis and isomerization of)
RN 139285-17-9 HCAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 5-(benzoylamino)-4,5-dihydro-1,3,4-triphenyl-, methyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



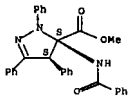
RN 145383-27-3 HCAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 5-(benzoylamino)-4,5-dihydro-4-(4-methoxyphenyl)-1,3-diphenyl-, methyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



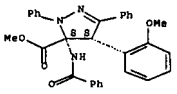
IT 129624-41-5P 145383-20-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and methanolysis of)
RN 129624-41-5 HCAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 5-(benzoylamino)-4,5-dihydro-1,3,4-triphenyl-, methyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



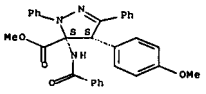
RN 145383-20-6 HCAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 5-(benzoylamino)-4,5-dihydro-4-(2-methoxyphenyl)-1,3-diphenyl-, methyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



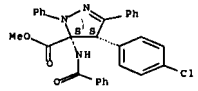
IT 145383-21-7P 145383-22-8P 145383-23-9P 145383-24-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by regioselective and stereoselective cycloaddn. of diphenylnitrilimine with Me β-aryl-N-benzoyl-α,β-didehydroalaninate)
RN 145383-21-7 HCAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 5-(benzoylamino)-4,5-dihydro-4-(4-methoxyphenyl)-1,3-diphenyl-, methyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



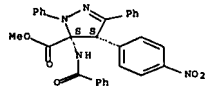
RN 145383-22-8 HCAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 5-(benzoylamino)-4-(4-chlorophenyl)-4,5-dihydro-1,3-diphenyl-, methyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



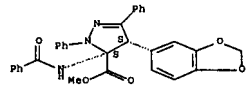
RN 145383-23-9 HCAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 5-(benzoylamino)-4,5-dihydro-4-(4-nitrophenyl)-1,3-diphenyl-, methyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

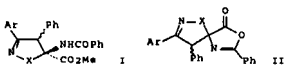


RN 145383-24-0 HCAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 4-(1,3-benzodioxol-5-yl)-5-(benzoylamino)-4,5-dihydro-1,3-diphenyl-, methyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L5 ANSWER 39 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1992:128760 HCAPLUS Full-text
DOCUMENT NUMBER: 116:128760
TITLE: On the synthesis of geminally functionalized heterocyclic aminocarboxylic acid esters
AUTHOR(S): Coutouli-Argyropoulou, E.; Thessalonikeos, E.
CORPORATE SOURCE: Lab. Org. Chem., Univ. Thessaloniki, Thessaloniki, 540 06, Greece
SOURCE: Journal of Heterocyclic Chemistry (1991), 28(8), 1945-8
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 116:128760
GI



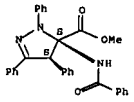
AB The title compds. I (X = O, Ar = mesityl, 2,6-Cl2C6H3; X = NPh, Ar = Ph, 4-MeC6H4, 4-ClC6H4) were easily prepared by two alternative procedures: 1,3-dipolar cycloaddn. to benzamidocinnamates prepared by methanolysis of the corresponding oxazolones or methanolysis of the spirooxazolones II, synthesized by 1,3-dipolar cycloaddn. to oxazolones. Both reaction sequences show the same stereo- and regioselectivity.

IT 129624-41-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and aromatization of)

RN 129624-41-5 HCAPLUS

CN 1H-Pyrazole-5-carboxylic acid, 5-(benzoylamino)-4,5-dihydro-1,3,4-triphenyl-, methyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

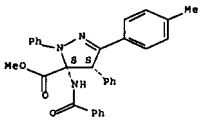


IT 139285-15-7P 139285-16-8P 139285-17-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 139285-15-7 HCAPLUS

CN 1H-Pyrazole-5-carboxylic acid, 5-(benzoylamino)-4,5-dihydro-3-(4-methylphenyl)-1,4-diphenyl-, methyl ester, cis- (9CI) (CA INDEX NAME)

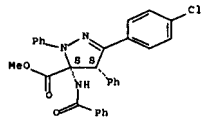
Relative stereochemistry.



RN 139285-16-8 HCAPLUS

CN 1H-Pyrazole-5-carboxylic acid, 5-(benzoylamino)-3-(4-chlorophenyl)-4,5-dihydro-1,4-diphenyl-, methyl ester, cis- (9CI) (CA INDEX NAME)

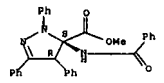
Relative stereochemistry.



RN 139285-17-9 HCAPLUS

CN 1H-Pyrazole-5-carboxylic acid, 5-(benzoylamino)-4,5-dihydro-1,3,4-triphenyl-, methyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L5 ANSWER 40 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1990:552311 HCAPLUS Full-text

DOCUMENT NUMBER: 113:152311

TITLE: 1,3-Dipolar cycloaddition reactions of 2-phenyl-4-arylideneoxazol-5(4H)-ones with nitrile imines. A reinvestigation of the regiochemistry of the 1,3-dipolar cycloaddition reactions of 2-phenyl-4-arylideneoxazol-5(4H)-ones with nitrile oxides

AUTHOR(S): Coutouli-Argyropoulou, Evdoxia; Argyropoulos, Nikolaos G.; Thessalonikeos, Elisavet

CORPORATE SOURCE: Dep. Chem., Univ. Thessaloniki, Thessaloniki, 54006, Greece

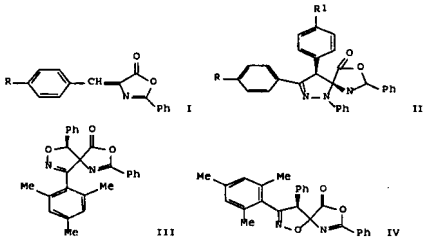
SOURCE: Journal of Chemical Research, Synopses (1990), (7), 202-3
CODEN: JRPSDC; ISSN: 0308-2342

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 113:152311

GI



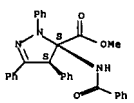
AB The title reaction of phenylarylideneoxazolones I (R = H, Me, MeO) with 4-R1C6H4C.tplbond.N+N-Ph (R1 = H, Me, Cl), generated from 4-R1C6H4CCl:NNHPh with Et3N, gave spiro[pyrazoline-oxazolin]ones II. The structure of II was supported by anal. and spectral data. The regiochem. of these cycloaddns. suggested that nitrile oxides might add in a similar fashion, thus, the nitrile oxide-cycloadduct previously assigned structure III was reexamd. and shown to be the regioisomer IV.

IT 129624-41-5P 129624-42-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 129624-41-5 HCAPLUS

CN 1H-Pyrazole-5-carboxylic acid, 5-(benzoylamino)-4,5-dihydro-1,3,4-triphenyl-, methyl ester, cis- (9CI) (CA INDEX NAME)

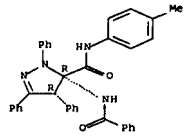
Relative stereochemistry.



RN 129624-42-6 HCAPLUS

CN 1H-Pyrazole-5-carboxamide, 5-(benzoylamino)-4,5-dihydro-N-(4-methylphenyl)-1,3,4-triphenyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L5 ANSWER 41 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1989:534747 HCAPLUS Full-text

DOCUMENT NUMBER: 111:134747

TITLE: Preparation and testing of heterocyclylcarbonylglutamides and - aspartamides as cholecystokinin antagonists

INVENTOR(S): Nadzan, Alex M.; Lin, Chun Wei; Kerwin, James F., Jr.

PATENT ASSIGNEE(S): Abbott Laboratories, USA

SOURCE: Eur. Pat. Appl., 68 pp.
CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 308885	A1	19890329	EP 1988-115462	19880921 <--
R: ES, GR				
US 4971978	A	19901120	US 1988-234525	19880822 <--
WO 8902431	A1	19890323	WO 1988-US3181	19880921 <--
W: JP				
RW: BE, CH, DE, FR, GB, IT, NL, SE				
US 5128346	A	19920707	US 1990-571945	19900823 <--

PRIORITY APPLN. INFO.: US 1987-99866 A 19870921
US 1988-234525 A 19880822

OTHER SOURCE(S): MARPAT 111:134747

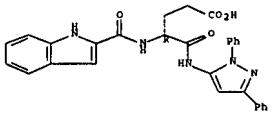
AB ArX1X2NR3 CH[(CH2)nR4] CONR1R2 [I; R1, R2 = H, C1-8 alkyl, cycloalkyl, alkenyl, cyanoalkyl, adamantyl, carbamoylalkyl, etc.; R2R2N = morpholino, pyrrolidinyl, piperazinyl, piperidino, etc.; R3 = H, alkyl, cycloalkyl, alkenyl, (substituted) arylalkyl, heterocyclylalkyl; R4 = tetrazolyl, acyl; Ar = heterocyclyl; X1 = (CH2)n, OCH2, SCH2, NH, (substituted) alkenyl; X2 = CO, CS, SO2; m = 0-4; n = 1-3], useful as cholecystokinin (CCK) antagonists, were prepared H-Glu(OBZl)-N[(CH2)2Me]2.HCl (preparation given) and N-methylmorpholine in DMF at 0° were treated successively with indole-2-carboxylic acid, 1-hydroxybenzotriazole, and 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide. The mixture was allowed to warm to room temperature and stirred overnight and the product was debenzylated with Pd/C/cyclohexadiene to give N-(2'-indolylcarbonyl)-L-glutamine di-N-pentylamide. I inhibit specific [125I]-Bolton-Hunter CCK-8 pancreatic receptor binding with IC50's of 5.4-820 nm.

IT 122667-84-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as cholecystokinin antagonist)

RN 122667-84-9 HCAPLUS

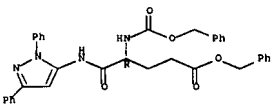
CN Pentanoic acid, 5-[(1,3-diphenyl-1H-pyrazol-5-yl)amino]-4-[(1H-indol-2-ylcarbonyl)amino]-5-oxo-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



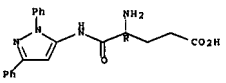
IT 122668-27-3P 122668-28-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for cholecystokinin antagonist)
RN 122668-27-3 HCAPLUS
CN Pentanoic acid, 5-[(1,3-diphenyl-1H-pyrazol-5-yl)amino]-5-oxo-4-[[(phenylmethoxy)carbonyl]amino]-, phenylmethyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



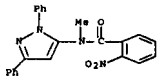
RN 122668-28-4 HCAPLUS
CN Pentanoic acid, 4-amino-5-[(1,3-diphenyl-1H-pyrazol-5-yl)amino]-5-oxo-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

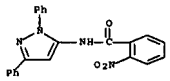


L5 ANSWER 42 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1986:439189 HCAPLUS Full-text
DOCUMENT NUMBER: 105:39189
TITLE: N-pyrazolyl-2-nitrobenzamides with antifungal activity
AUTHOR(S): Daidone, G.; Plescia, S.; Raffa, D.; Sprio, V.; Milici, M.
CORPORATE SOURCE: Ist. Chim. Farm. Tossicol., Univ. Palermo, Palermo, Italy
SOURCE: Farmaco, Edizione Scientifica (1986), 41(5), 408-16
CODEN: FRPSAX; ISSN: 0430-0920
DOCUMENT TYPE: Journal
LANGUAGE: Italian

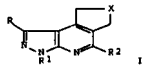
AB N-Pyrazolyl-2-nitrobenzamides substituted on the pyrazole nucleus were screened for antifungal activity against Candida albicans and Cryptococcus neoformans. Min. inhibitory concns. for 14 tested compds. ranged 20-70 and 20-80 μg/mL for the 2 species, resp. However, the species differed considerably in their sensitivity to individual compds. The presence of both a secondary amide function and a nitroso group conferred increased activity, particularly with respect to C. albicans. Introduction of a Ph group into the pyrazole nucleus increased activity, presumably due to enhanced lipophilicity.
IT 69730-12-7
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(fungicidal activity of)
RN 69730-12-7 HCAPLUS
CN Benzamide, N-(1,3-diphenyl-1H-pyrazol-5-yl)-N-methyl-2-nitro- (9CI) (CA INDEX NAME)



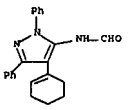
IT 69730-02-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and fungicidal activity of)
RN 69730-02-5 HCAPLUS
CN Benzamide, N-(1,3-diphenyl-1H-pyrazol-5-yl)-2-nitro- (9CI) (CA INDEX NAME)



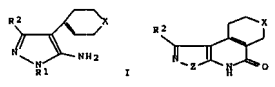
L5 ANSWER 43 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1986:28553 HCAPLUS Full-text
DOCUMENT NUMBER: 104:28553
TITLE: Synthesis and analgesic activity of new tricyclic pyrazolo[3,4-b]pyridine
AUTHOR(S): Winters, G.; Schiatti, P.; Selva, D.
CORPORATE SOURCE: Lepetit Res. Lab., Milan, Italy
SOURCE: Farmaco, Edizione Scientifica (1985), 40(11), 845-53
CODEN: FRPSAX; ISSN: 0430-0920
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



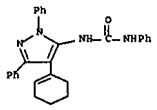
AB Ten title compds. (I; R = R1 = Me or Ph; R2 = H, Me, or CH2Ph; X = (CH2)n, CH2CH(Me), or CH(Me)CH2; n = 1-3) were prepared, in 2 steps starting from 5-amino-4-(1-cycloalkenyl)pyrazoles, and tested for analgesic, anti-inflammatory, and antipyretic active in mice and rats. 6,7,8,9-Tetrahydro-1,3-dimethyl-3H-pyrazolo[3,4-c]isoquinoline (I; R = R1 = Me; R2 = H, X = CH2) [91623-78-8] showed strong anti-inflammatory and analgesic activity with no ulcerogenesis at doses up to 100 mg/kg; this compound was also moderately antipyretic. The LD50 of I in mice is also given.
IT 99699-95-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)
RN 99699-95-3 HCAPLUS
CN Formamide, N-[4-(1-cyclohexen-1-yl)-1,3-diphenyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)



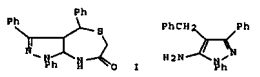
L5 ANSWER 44 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1985:437407 HCAPLUS Full-text
DOCUMENT NUMBER: 103:37407
TITLE: Easy synthesis of new ring-fused pyridones from heteroaromatic β-vinylamines
AUTHOR(S): Winters, G.; Sala, A.; De Paoli, A.; Ferri, V.
CORPORATE SOURCE: Res. Lab., DOW-Lepetit, Milan, I-20158, Italy
SOURCE: Synthesis (1984), (12), 1052-4
CODEN: SYNTBF; ISSN: 0039-7881
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 103:37407
GI



AB Cyclization of pyrazoles I (R1, R2 = Me, Ph; X = -, CH2, CH2CH2, NAc, NMe) with RNCO (R = Ph, Et) gave 75-98% cycloalkapyrazolopyridines II (Z = NR1). Similarly prepared were II (Z = O).
IT 97139-76-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)
RN 97139-76-9 HCAPLUS
CN Urea, N-[4-(1-cyclohexen-1-yl)-1,3-diphenyl-1H-pyrazol-5-yl]-N'-phenyl- (9CI) (CA INDEX NAME)

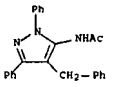


L5 ANSWER 45 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1984:472700 HCAPLUS Full-text
DOCUMENT NUMBER: 101:72700
TITLE: Synthesis of 1,3,4-triphenyl-1H-pyrazolo[3,4-e][1,4]thiazepin-7-one
AUTHOR(S): Vartanyan, R. S.; Gyul'budagyan, A. L.; Vartanyan, S. A.
CORPORATE SOURCE: Inst. Tonkoi Org. Khim. im. Mndzhoyana, Yerevan, 375014, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1984), (4), 464-5
CODEN: KGSSAQ; ISSN: 0453-8234
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 101:72700
GI



AB Reaction of 1,3-diphenyl-5-pyrazolamine with BzH gave the Schiff base, which was cyclized with HSCH2CO2H to give the title compound (I); desulfurization of I with Raney Ni gave 5-acetamido-4-benzyl-1,3- diphenylpyrazole, which was deacetylated to give the amine II.
IT 91255-66-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deacetylation of)
RN 91255-66-2 HCAPLUS
CN Acetamide, N-[1,3-diphenyl-4-(phenylmethyl)-1H-pyrazol-5-yl]- (9CI) (CA

INDEX NAME)



L5 ANSWER 46 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1982:217756 HCAPLUS Full-text
DOCUMENT NUMBER: 96:217756
TITLE: Aminopyrazoles. II. Synthesis of pyrazolo[3,4,-b]pyridines via Vilsmeier-Haack reaction of 5-acetaminopyrazoles
AUTHOR(S): Simay, Antal; Takacs, Kalman; Toth, Laszlo
CORPORATE SOURCE: Res. Dep., Chinoin Pharm. Chem. Works, Budapest, Hung.
SOURCE: Acta Chimica Academiae Scientiarum Hungaricae (1982), 109(2), 175-87
CODEN: ACASA2; ISSN: 0001-5407
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 96:217756
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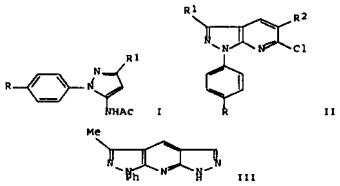
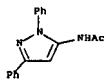
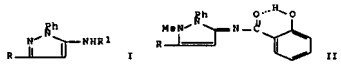


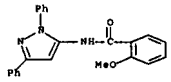
AB Vilsmeier-Haack reaction of pyrazoles I (R = H, Cl, NO2, R1 = H; R = H, R1 = Me, Ph) gave 8-25% II (R2 = H) and 35-53% II (R2 = CHO). II (R = H, R1 = Me, R2 = CHO) was subjected various reactions, including the formation of III.
IT 69730-07-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(Vilsmeier-Haack reaction of)
RN 69730-07-0 HCAPLUS
CN Acetamide, N-(1,3-diphenyl-1H-pyrazol-5-yl)- (9CI) (CA INDEX NAME)



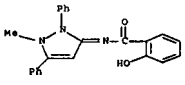
L5 ANSWER 47 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1981:569066 HCAPLUS Full-text
DOCUMENT NUMBER: 95:169066
TITLE: Studies on the synthesis of heterocyclic compounds. Part VI. The action of methyl salicylate on some 5-aminopyrazoles
AUTHOR(S): Daidone, Giuseppe; Plescia, Salvatore
CORPORATE SOURCE: Ist. Chim. Farm. Tossicol., Univ. Palermo, Palermo, 32-90123, Italy
SOURCE: Journal of Heterocyclic Chemistry (1981), 18(4), 747-50
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 95:169066
GI



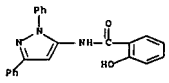
AB Refluxing 5-aminopyrazoles I (R = H, Me, Ph; R1 = H) with o-HOC6H4CO2Me gave I (R1 = o-MeOC6H4CO, Me) and II.
IT 79442-81-2P 79442-84-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)
RN 79442-81-2 HCAPLUS
CN Benzamide, N-(1,3-diphenyl-1H-pyrazol-5-yl)-2-methoxy- (9CI) (CA INDEX NAME)



RN 79442-84-5 HCAPLUS
CN Benzamide, N-(1,2-dihydro-2,5-diphenyl-1-methyl-3H-pyrazol-3-ylidene)-2-hydroxy- (9CI) (CA INDEX NAME)

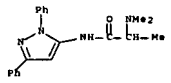


IT 70803-13-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with Me salicylate)
RN 70803-13-3 HCAPLUS
CN Benzamide, N-(1,3-diphenyl-1H-pyrazol-5-yl)-2-hydroxy- (9CI) (CA INDEX NAME)

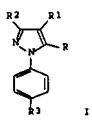


L5 ANSWER 48 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1981:538523 HCAPLUS Full-text
DOCUMENT NUMBER: 95:138523
TITLE: Stability of packaged solid dosage forms. V. Prediction of the effect of aging on the disintegration of packaged tablets influenced by moisture and heat
AUTHOR(S): Nakabayashi, Kiyoshi; Shimamoto, Tsugio; Mima, Hiroyuki; Okada, Jutaro
CORPORATE SOURCE: Cent. Res. Div., Takeda Chem. Ind., Ltd., Osaka, 532, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1981), 29(7), 2051-6
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The effects of moisture and temperature on the disintegration time of a tablet containing gelatin as binder were investigated under accelerated conditions. The higher the ambient temperature and the moisture content of the tablet, the longer the disintegration time. Among several kinetic models investigated, a half-order reaction model was most suitable, when the ratio of the disintegration time of the aged samples to that of the initial ones was taken as a variable to be predicted. The effects of moisture and heat on the disintegration time ratio were analyzed by a multiple regression technique on the basis of the Carstensen equation. In order to estimate the effect of aging on the disintegration time ratio, tablets in several kinds of moisture-semipermeable packages, including an overwrapped package, were examined in artificial climate labs. The effect of aging could be predicted by an iterative calcn. through a math. model in which the kinetics of the increase in the disintegration time ratio was combined with the moisture permeability of the packages. The simulated values could represent the observed data fairly well, although the confidence intervals of the predicted values were rather wide, owing to variances of the exptl. data obtained.
IT 20170-20-1
RL: BIOL (Biological study)
(tablet, disintegration of, moisture and storage temperature effect on)
RN 20170-20-1 HCAPLUS

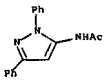
CN Propanamide, 2-(dimethylamino)-N-(1,3-diphenyl-1H-pyrazol-5-yl)- (9CI) (CA INDEX NAME)



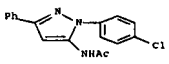
L5 ANSWER 49 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1981:442979 HCAPLUS Full-text
DOCUMENT NUMBER: 95:42979
TITLE: Vilsmeier-Haack reaction of 5-amino- and 5-acylaminopyrazoles
AUTHOR(S): Simay, A.; Takacs, K.; Horvath, K.; Dvortsak, P.
CORPORATE SOURCE: Res. Dep., Chinoin Pharm. Chem. Works, Budapest, Hung.
SOURCE: Acta Chimica Academiae Scientiarum Hungaricae (1980), 105(2), 127-39
CODEN: ACASA2; ISSN: 0001-5407
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 95:42979
GI



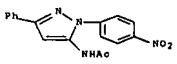
AB Vilsmeier-Haack reaction of aminopyrazoles I (R = NH2, R1 = H, R2 = H, Me, Ph, R3 = H, Cl, NO2, Me, OMe) gave I (R = N:CHNR42, R1 = CHO, NR42 = NMe2, piperidino). The intermediates I (R = N:CHNR42, R1 = H, CH:N+R42X-, X = Cl, PO2Cl2, ClO4) were isolated. I (R = NHCHO, NHAc, NHBz, R1 = H) similarly gave I (R = N:CHNR42, R1 = CHO, H). I (R = N:CHNMe2, R1 = CHO) were converted into I (R1 = CH:NPh, CH:NNHPh, CH:NNHCONH2, CH:NNHCSNH2) and I [RR1 = N:CHN:CH, N:CHN(O):CH].
IT 69730-07-0P 77746-65-1P 77746-87-3P
77746-90-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and Vilsmeier-Haack reaction of)
RN 69730-07-0 HCAPLUS
CN Acetamide, N-(1,3-diphenyl-1H-pyrazol-5-yl)- (9CI) (CA INDEX NAME)



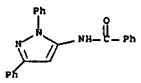
RN 77746-85-1 HCAPLUS
CN Acetamide, N-[1-(4-chlorophenyl)-3-phenyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)



RN 77746-87-3 HCAPLUS
CN Acetamide, N-[1-(4-nitrophenyl)-3-phenyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

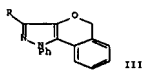


RN 77746-90-8 HCAPLUS
CN Benzamide, N-(1,3-diphenyl-1H-pyrazol-5-yl)- (9CI) (CA INDEX NAME)



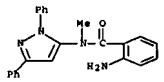
L5 ANSWER 50 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1981:121395 HCAPLUS Full-text
DOCUMENT NUMBER: 94:121395
TITLE: Studies on the synthesis of heterocyclic compounds. Part IV. Further investigation of the Pschorr reaction with some pyrazole derivatives
AUTHOR(S): Daidone, Giuseppe; Plescia, Salvatore; Fabra, Jole
CORPORATE SOURCE: Ist. Chim. Farm. Tossicol., Univ. Via Archirafi, Palermo, 32-90123, Italy
SOURCE: Journal of Heterocyclic Chemistry (1980), 17(7), 1409-11
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal

LANGUAGE: English
OTHER SOURCE(S): CASREACT 94:121395
GI



III

AB Thermal decomposition of the diazonium sulfate derived from N-methyl-(1-phenyl-3-methylpyrazol-5-yl)-2-aminobenzamide afforded products formulated as 1-phenyl-3-methyl[2]benzopyrano[4,3-c]pyrazol-5-one (yield 10%), 1,4-dimethyl-3-phenylpyrazolo[3,4-c]isoquinolin-5-one (yield 10%), N-methyl-(1-phenyl-3-methylpyrazol-5-yl)-2-hydroxybenzamide (yield 8%) and 4'-hydroxy-2,3'-dimethyl-1'-phenylspiro[isoindoline-1,5'-[2]pyrazolin]-3-one (I) (yield 20%). Decomposition of the diazonium sulfate derived from N-methyl-(1,3-diphenylpyrazol-5-yl)-2-aminobenzamide gave products formulated as 7,9-dimethyldibenzo[e,g]pyrazolo[1,5- a][1,3]diazocin-10(9H)-one (yield 8%), 4-methyl-1,3-diphenylpyrazolo[3,4- c]isoquinolin-5-one (yield 7%) and 4'-hydroxy-2-methyl-1',3'-diphenylspiro[isoindoline-1,5'-[2]pyrazolin]-3-one (II) (yield 10%). The spiro compds. I and II underwent thermal and acid-catalyzed conversion into the hitherto unknown 2-benzopyrano[4,3-c]pyrazole ring system III (R = Me, Ph) in good yield.
IT 69730-14-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of diazonium sulfate from, decomposition of)
RN 69730-14-9 HCAPLUS
CN Benzamide, 2-amino-N-(1,3-diphenyl-1H-pyrazol-5-yl)-N-methyl- (9CI) (CA INDEX NAME)

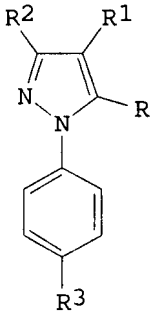


=> log hold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	341.50	514.26
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-39.00	-39.00

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 09:43:53 ON 23 MAY 2007

L5 ANSWER 49 OF 92 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1981:442979 HCAPLUS <<LOGINID::20070523>>
DOCUMENT NUMBER: 95:42979
TITLE: Vilsmeier-Haack reaction of 5-amino- and 5-acylaminopyrazoles
AUTHOR(S): Simay, A.; Takacs, K.; Horvath, K.; Dvortsak, P.
CORPORATE SOURCE: Res. Dep., Chinoin Pharm. Chem. Works, Budapest, Hung.
SOURCE: Acta Chimica Academiae Scientiarum Hungaricae (1980), 105(2), 127-39
CODEN: ACASA2; ISSN: 0001-5407
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 95:42979
GI

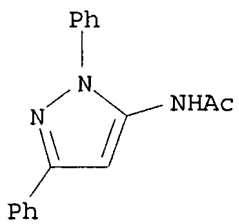


I

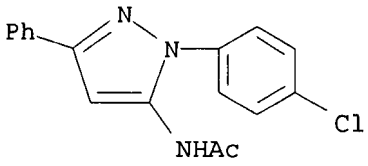
AB Vilsmeier-Haack reaction of aminopyrazoles I (R = NH2, R1 = H, R2 = H, Me, Ph, R3 = H, Cl, NO2, Me, OMe) gave I (R = N:CHNR42, R1 = CHO, NR42 = NMe2, piperidino). The intermediates I (R = N:CHNR42, R1 = H, CH:N+R42X-, X = Cl, PO2Cl2, ClO4) were isolated. I (R = NHCHO, NHAc, NHBz, R1 = H) similarly gave I (R = N:CHNR42, R1 = CHO, H). I (R = N:CHNMe2, R1 = CHO) were converted into I (R1 = CH:NPh, CH:NNHPh, CH:NNHCONH2, CH:NNHCSNH2) and I [RR1 = N:CHN:CH, N:CHN(O):CH].

IT 69730-07-0P 77746-85-1P 77746-87-3P
77746-90-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and Vilsmeier-Haack reaction of)

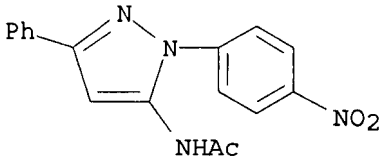
RN 69730-07-0 HCAPLUS
CN Acetamide, N-(1,3-diphenyl-1H-pyrazol-5-yl)- (9CI) (CA INDEX NAME)



RN 77746-85-1 HCAPLUS
CN Acetamide, N-[1-(4-chlorophenyl)-3-phenyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)



RN 77746-87-3 HCAPLUS
CN Acetamide, N-[1-(4-nitrophenyl)-3-phenyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)



RN 77746-90-8 HCAPLUS
CN Benzamide, N-(1,3-diphenyl-1H-pyrazol-5-yl)- (9CI) (CA INDEX NAME)